Doctoral Thesis

Circular bioeconomy applications in chemical engineering

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by

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Vienna, September 2023

Fernando Ramonet Marqués

Abstract

The transition to the bioeconomy requires the synergic integration of different technologies and existing industries. This thesis explores various applications of circular bioeconomy in chemical engineering, covering several key areas. Firstly, it presents a circular economy model designed explicitly for arid coastal regions with water scarcity by strategically incorporating existing technologies in these regions. The thesis then explores the potential utilization of unutilized carbon dioxide (CO_2) from biomethane plants for greenhouse crop farming. A growing and essential sector in the bioeconomy is the biorefinery industry, where bioreactors play a critical role as a key technology and essential component.

Computational fluid dynamics (CFD) has emerged as a crucial tool for designing, optimizing, and scaling bioreactors. In this thesis, CFD is employed to study the hydrodynamic behavior of pneumatic-driven bioreactors and the power consumption of mechanical mixing reactors. An emphasis is put on Internal Loop Air Lift Reactors (ILALRs). Global hydrodynamics is studied for different vessel shapes and multi-stage ILALRs with single, double, and triple draft tube configurations. Additionally, the impact of varying double-draft tube configurations on reactor performance and the design of draft tubes are thoroughly explored.

The optimization of microorganism growth and productivity in bioreactors heavily relies on the mixing strategy. In mechanical stirred systems such as the continuously stirred tank reactor (CSTR), power consumption is one of the main industrial concerns. Therefore, the efficient use of power in these systems is crucial for optimizing operational costs and ensuring sustainable operation. To assess energy efficiency, power consumption is compared among different stirring systems in CSTRs. This comparison is based on power numbers derived from both experimental measurements and simulated torque data, providing valuable insights into the performance of the stirring systems.

Continuing the exploration, the thesis advances an innovative concept for a two-stage covered lagoon anaerobic digester that integrates wind energy. This innovative proposition holds the potential to enhance the efficiency of anaerobic digestion processes while concurrently reducing capital expenditures, making it applicable to a wide range of scales, from small to large. Furthermore, a comprehensive safe-by-design framework is introduced, aiming to enhance safety considerations within biorefineries. This proposed framework aims to create a safer working environment while promoting sustainable practices within the industry.

The insights obtained from this thesis, encompassing the design and optimization of bioreactors and various chemical engineering applications for the emerging bioeconomy, hold significant promise for advancing sustainable practices, driving innovation, and fostering economic growth in diverse industries.

Kurzfassung

Der Übergang zur Bioökonomie erfordert die synergetische Integration verschiedener Technologien und bestehender Industrien. In dieser Arbeit werden verschiedene Anwendungen der Bio-Kreislaufwirtschaft in der chemischen Verfahrenstechnik untersucht, wobei mehrere Schlüsselbereiche abgedeckt werden. Zunächst wird ein Kreislaufwirtschaftsmodell vorgestellt, das speziell für trockene Küstenregionen mit Wasserknappheit entwickelt wurde, indem bestehende Technologien in diesen Regionen strategisch eingebunden werden. Anschließend wird das Potenzial der Nutzung von ungenutztem Kohlendioxid (CO_2) aus Biomethananlagen für den Anbau von Gewächshauspflanzen untersucht. Ein wachsender und wichtiger Sektor der Bioökonomie ist die Bioraffinerie-Industrie, in der Bioreaktoren als Schlüsseltechnologie und wesentliche Komponente eine entscheidende Rolle spielen.

Die numerische Strömungsmechanik (CFD) hat sich als entscheidendes Werkzeug für die Auslegung, Optimierung und Skalierung von Bioreaktoren erwiesen. In dieser Arbeit wird CFD eingesetzt, um das hydrodynamische Verhalten von pneumatisch angetriebenen Bioreaktoren und den Energieverbrauch von mechanischen Mischreaktoren zu untersuchen. Ein Schwerpunkt liegt dabei auf Internal Loop Air Lift Reactors (ILALRs). Die globale Hydrodynamik wird für verschiedene Gefäßformen und mehrstufige ILALRs mit einfacher, doppelter und dreifacher Saugrohrkonfiguration untersucht. Darüber hinaus werden die Auswirkungen unterschiedlicher Doppelzugrohrkonfigurationen auf die Reaktorleistung und die Auslegung der Zugrohre eingehend untersucht.

Die Optimierung des Wachstums und der Produktivität von Mikroorganismen in Bioreaktoren hängt stark von der Mischstrategie ab. Bei mechanisch gerührten Systemen wie dem kontinuierlichen Rührkesselreaktor (CSTR) ist der Stromverbrauch eines der wichtigsten industriellen Anliegen. Daher ist die effiziente Nutzung der Energie in diesen Systemen entscheidend für die Optimierung der Betriebskosten und die Gewährleistung eines nachhaltigen Betriebs. Um die Energieeffizienz zu bewerten, wird der Energieverbrauch verschiedener Rührsysteme in CSTRs miteinander verglichen. Dieser Vergleich basiert auf Leistungszahlen, die sowohl aus experimentellen Messungen als auch aus simulierten Drehmomentdaten abgeleitet wurden und wertvolle Einblicke in die Leistung der Rührsysteme liefern.

Im weiteren Verlauf der Arbeit wird ein innovatives Konzept für einen zweistufigen, überdachten anaeroben Lagunenfermenter vorgestellt, der Windenergie integriert. Dieser innovative Vorschlag birgt das Potenzial, die Effizienz anaerober Vergärungsprozesse zu verbessern und gleichzeitig die Investitionskosten zu senken, so dass er in einem breiten Spektrum von kleinen bis großen Anlagen eingesetzt werden kann. Darüber hinaus wird ein umfassender Rahmen für eine sichere Auslegung eingeführt, der die Sicherheitsaspekte in Bioraffinerien verbessern soll. Der vorgeschlagene Rahmen zielt darauf ab, ein sichereres Arbeitsumfeld zu schaffen und gleichzeitig nachhaltige Praktiken in der Branche zu fördern.

Die in dieser Arbeit gewonnenen Erkenntnisse, die die Konstruktion und Optimierung von Bioreaktoren und verschiedene verfahrenstechnische Anwendungen für die aufstrebende Bioökonomie umfassen,

sind vielversprechend, um nachhaltige Praktiken voranzutreiben, Innovationen voranzutreiben und das Wirtschaftswachstum in verschiedenen Branchen zu fördern.

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I would like to begin by expressing my heartfelt gratitude to God, as well as to my parents and my wife, for their unwavering love, support, and encouragement throughout my journey in completing this thesis.

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I would like to express my appreciation to all my AgRefine colleagues, especially to Mayuki, who provided invaluable assistance throughout this project.

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List of appended publications

Journal publications

This Dissertation is grounded on the following publications. Certain specific sections and results from these publications are included in this document to provide context. However, the full description and results can be found in the respective publications for a comprehensive understanding and detailed information. The publications are referenced in the text using the assigned numerals listed below.

Journal Publication 1	Mayuki Cabrera-González, Fernando Ramonet, Michael Harasek. Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions. Land 2022, 11, 1506. DOI: 10.3390/land11091506
Journal Publication 2	Fernando Ramonet, Cristian Jordan, Bahram Haddadi, Michael Harasek. Anaerobic Digestion as a Carbon Capture, Storage, and Utilization Technology, Chemical Engineering Transactions, 96, 49-54, 2022. DOI: 10.3303/CET2296009
Journal Publication 3	Fernando Ramonet, Bahram Haddadi, Cristian Jordan, Michael Harasek. Modelling and Design of Optimal Internal Loop Air-Lift Reactor Configurations Through Computational Fluid Dynamics. Chemical Engineering Transactions, 94, 817-822, 2022. DOI: 10.3303/CET2294136
Journal Publication 4	Fernando Ramonet, Bahram Haddadi, Michael Harasek. Optimal Design of Double Stage Internal Loop Air-Lift Bioreactor. Energies, 16(7), 3267. DOI: 10.3390/en16073267
Journal Publication 5	Fernando Ramonet, Mara Kovacevic, Bahram Haddadi, Cristian Jordan, Michael Harasek. Bioreactor Mixing: A Comparison of Computational Fluid Dynamics and Experimental Approaches in the Pursuit of Sustainable Bioprocessing for the Bioeconomy. Special Issue: E2DT 2023 - Chemical Engineering Transactions. Status: submitted, June 2023

Unpublished Manuscripts

The two manuscripts presented here are an essential component of the thesis and are currently undergoing finalization. While the manuscripts are still being completed, this document provides an overview of the important findings and results.

Journal Publication 6	Fernando Ramonet, Tim Gleeson, Micheal Galvin, Bahram Haddadi, Michael Harasek. Anaerobic Digestion as A Tool to Mitigate Greenhouse Gas Emissions from Animal Slurries. Status: Manuscript, in writing
Journal Publication 7	Fernando Ramonet, Mayuki Cabrera-González, Michael Harasek. Promoting Safe Operations in Biorefineries: A Comprehensive Safe by Design Framework. Status: Manuscript, in writing

Conference publications

The following conference publications served as crucial proof of concept, demonstrating how the scientific community responded to the topics and providing valuable insights and feedback.

Conference Publication 1	Fernando Ramonet, Bahram Haddadi, Markus Bosenhofer, Michael Harasek. Modelling of Multi-Stage Internal Loop Air Lift Bioreactor Utilizing Computational Fluid Dynamics, 7th Minisymposium Verfahrenstechnik and 8th Partikelforum, BOKU, Vienna, April 13th – 14th, 2023, ISBN: 978-3-900397-08-1.
Conference Poster 1	Mayuki Cabrera-González, Fernando Ramonet, Michael Harasek. Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions. Circular@WUR: Living within planetary boundaries, Wageningen University and Research, Wageningen, 11-13 April, 2022. DOI: 10.13140/RG.2.2.21658.11200
Conference Poster 2	Fernando Ramonet, Michael Harasek. Modelling Study on the Co-Digestion of Nopal Cladodes with Farm Manures. 30th European Biomass Conference & Exhibition (EUBCE2022).Paris, France (online), 9-12 May, 2022, ISBN: 978-88-89407-22-6
Conference Poster 3	Fernando Ramonet, Bahram Haddadi, Michael Harasek. Modelling And Characterization Of Internal Loop Air Lift Bioreactor Configurations Through Computational Fluid Dynamics. Biorefine Conference 'The role of biorefineries in European agriculture'. Ghent, Belgium, 30-31 May, 2022. DOI: 10.13140/RG.2.2.16383.89765

Public reports

Dissemination to the general public and policy makers played a significant role in sharing the findings and outcomes of the research. The public reports were designed to effectively communicate the key insights, implications, and recommendations to a broader audience, including individuals, organizations, and policy makers involved in shaping and implementing relevant policies and initiatives.

Public Report 1	Srija Balachandran, Mariana Cerca, Rushab Chopda, Fernando Ramonet, Charlene Vance, Steven De Meester, Michael Harasek Erik Meers, Fionnuala Murphy, Ana Robles-Aguilar. State-of-the-art Report on Anaerobic Digestion and Biorefinery Systems Level Design. European Comission. Reference Ares(2021)2235935 - 31/03/2021.
Public Report 2	Fernando Ramonet, Michael Harasek. CFD optimisation and analysis of existing AD and Biorefineries Report. European Comission. Reference Ares(2021)7353824 - 29/11/2021.
Public Report 3	Fernando Ramonet, Michael Harasek. Geometry and CFD results for AD retrofit and TPB up scaling Report. European Comission. Submitted on February 7, 2023.

Author’s Contributions

Journal publications

Journal Publication 1	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Mayuki Cabrera-González: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Michael Harasek: supervision, project administration, funding acquisition.
Journal Publication 2	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Cristian Jordan: supervision. Bahram Haddadi: supervision. Michael Harasek: supervision, project administration, funding acquisition.
Journal Publication 3	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Cristian Jordan: supervision. Bahram Haddadi: supervision. Michael Harasek: conceptualization, supervision, project administration, funding acquisition.
Journal Publication 4	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Bahram Haddadi: supervision. Michael Harasek: supervision, project administration, funding acquisition.
Journal Publication 5	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Mara Kovacevic: conceptualization, methodology. Cristian Jordan: conceptualization, supervision. Bahram Haddadi: supervision. Michael Harasek: supervision, project administration, funding acquisition.
Journal Publication 6	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Tim Gleeson: conceptualization. Micheal Galvin: conceptualization. Bahram Haddadi: supervision. Michael Harasek: supervision, project administration, funding acquisition.
Journal Publication 7	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Mayuki Cabrera-González: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Michael Harasek: supervision, project administration, funding acquisition.

Conference publications

Conference Publication 1	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization., Markus Bosenhofer: conceptualization, methodology. Bahram Haddadi: supervision. Michael Harasek: supervision, project administration, funding acquisition.
Conference Poster 1	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Mayuki Cabrera-González: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Michael Harasek: supervision, project administration, funding acquisition.
Conference Poster 2	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Michael Harasek: supervision, project administration, funding acquisition.
Conference Poster 3	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization. Bahram Haddadi: supervision. Michael Harasek: supervision, project administration, funding acquisition.

Public reports

Public Report 1	Fernando Ramonet, Srija Balachandran, Mariana Cerca, Rushab Chopda, Charlene Vance: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization., Michael Harasek, Steven De Meester, Erik Meers, Fionnuala Murphy, Ana Robles-Aguilar: supervision, project administration, funding acquisition.
Public Report 2	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization., Michael Harasek: supervision, project administration, funding acquisition.
Public Report 3	Fernando Ramonet: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization., Michael Harasek: supervision, project administration, funding acquisition.

Chapter 1. Introduction and motivation

“Human activities, principally through emissions of Green-House Gases (GHG), have unequivocally caused global warming” (IPCC, 2023). According to the Intergovernmental Panel for Climate Change (IPCC), due to the unsustainable utilization of energy and land, changes in land use, lifestyles, and patterns of consumption of individuals, countries, and regions, the global surface temperature has increased by 1.1 °C in 2011–2020, with respect to the 1850–1900 levels (IPCC, 2023).

The Paris Agreement (United Nations, 2016) has been a steppingstone for international cooperation on climate change as 195 countries (United Nations, 2023) agreed on a global goal of limiting global warming below 2 °C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5 °C above pre-industrial levels.

Significant changes are necessary to combat the rising global temperatures, as highlighted by a survey study published in the journal Nature (Tollefson, 2021). According to the survey (Tollefson, 2021), a considerable number of the authors involved in the 2021 IPCC report, 92 out of 233 surveyed anonymously, believe that achieving the 1.5 °C target is unlikely without changes to current norms, practices, and technologies.

To address this issue, the European Union has launched several initiatives, including the Green Deal, European Bioeconomy Strategy, Circular Economy Action Plan, Clean Energy for All Europeans Package, European Climate Law, Farm to Fork Strategy, and the EU Biodiversity Strategy for 2030, among others. These initiatives aim to reduce carbon emissions, promote sustainable agriculture and energy, and encourage a circular economy, all of which are crucial in achieving a more environmentally friendly future.

The Green Deal and the European Bioeconomy Strategy are among the key initiatives that are crucial in achieving the EU's carbon neutrality target by 2050. With the EU Bioeconomy Strategy at the forefront, research is increasingly focused on the potential of biomass as well as the tools used to convert it, including biorefineries and bioreactors, which are considered key technologies in this field. These technologies play a vital role in transforming biomass into a wide range of products. By doing so, they offer immense potential to support the development of a sustainable and circular bioeconomy, while reducing dependence on non-renewable resources and addressing environmental challenges like climate change and resource scarcity.

In order to shift from an economy based on oil to one based on biomass, it is necessary to develop flexible biorefineries that can be integrated with existing industrial infrastructure, such as biogas plants. According to Cherubini et al. (2009), existing industrial infrastructure can be classified for its suitability to be retrofitted into biorefineries according to their type of products, feedstocks, transformation processes, and the platforms they use. Utilizing this classification, biorefineries can be integrated into existing infrastructure.

The circular bioeconomy has emerged as a circular production method based on biomass resources, facilitated by biorefineries and bioreactors. This approach makes carbon sequestration from biomass sources possible, reducing greenhouse gas emissions and decreasing our dependence on oil-based products. In addition, responsible farming practices like sequential cropping (Magnolo et al., 2021) are promoted while taking into account ecosystem protection. As a result, sustainable biomass utilization, carbon sequestration, and responsible farming practices have gained significant importance in the development of the circular bioeconomy, further highlighting its potential to address environmental challenges and promote a sustainable and circular economy.

The European Commission has funded several projects with Horizon 2020 to promote the circular bioeconomy. One of these projects is the AgRefine project, which focuses on developing advanced biorefinery technologies for green and algal biorefineries. The aim is to train the next generation of bioeconomy leaders by creating new and optimizing current agri-resource and agri-waste valorization pathways. The project consists of 15 highly interdisciplinary and inter-sectoral Ph.D. projects, each specializing in specific aspects of the bioeconomy. The researchers were trained in several cross-cutting, multi-disciplinary, and highly interdisciplinary advanced technical subject areas, including chemical and process engineering, biological science, life cycle assessment, and economics. The project also aims to promote sustainable value chain creation and combined evaluation of legislation and policy with industry-led innovation of AgRefine technology. The project's specific objectives include creating a three-phase reactor technology to implement AgRefine's valorization cascade, developing an entire supply chain sustainability plan, and creating economically robust supply chains and sound business models.

The AgRefine project is organized into three distinct work packages (WPs) to achieve its objectives. The first work package (WP1) focuses on developing technology for creating a three-phase reactor system that can optimize the production of high-value products from biomass. This includes the development of a whole-cell biosensor platform to identify key-performance indicators in real-time, as well as the screening, identification, and genetic engineering of microorganisms to remove contaminants in the third phase of the reactor. The second work package (WP2) is focused on systems-level design to ensure the environmental and social sustainability of the AgRefine bioeconomy. This includes the development of supply chain management strategies, retrieving mineral nutrients from processed biomass, and using optimized CFD to improve plant retrofitting and upscaling. Finally, the third work package (WP3) is focused on value chains, including the development of supply chain sustainability plans and the creation of economically robust supply chains and business models. This includes the identification of innovative business models for the AgRefine sector and the design of governance arrangements to encourage responsive innovation and policy frameworks that support the development of AgRefine technology.

Overall, the AgRefine project is an ambitious and innovative initiative to develop advanced biorefinery technologies for the “agri-bioeconomy” industry. By providing Early Stage Researchers (ESRs) with the necessary skills and knowledge, the project aims to train the next generation of bioeconomy leaders and position Europe as a global leader in this field. The project has the potential to create significant economic, social, and environmental benefits, and its outcomes will be closely watched by industry stakeholders, policymakers, and researchers alike.

This thesis is framed on the AgRefine project's WP2 scope, which, as mentioned above, focuses on system-level design. The sub-project of which this thesis is part is titled "Computational Fluid Dynamics (CFD) Analysis and Retrofit of Existing Anaerobic Digestion (AD) and Biorefineries," and the objective is to use optimized CFD to improve the geometric and operational aspects of biogas plants and Three Phase Bioreactor (TPB) systems. The secondary objectives include developing modeling concepts based on the Design of Experiments to improve the geometric design and find optimal operating conditions under design constraints. The project also aims to disseminate an open-source CFD toolbox for the flow investigation of TPB systems.

Several actors will play a key role in the transition to the circular bioeconomy. Some of these actors are chemical engineers who design, operate, and optimize biochemical, chemical, petrochemical, and pharmaceutical plants. Chemical engineers are devoted to their role in developing a sustainable future. In 1997, eighteen professional chemical engineers' societies around the world signed the London Communiqué, promising to use their skills to improve the quality of life, foster employment, advance economic and social development and protect the environment, all with the goal of making the world a better place for future generations (Perkins, 2003).

This thesis proposes developing a new circular bioeconomy model (Journal Publication 1) and analyses the different technologies that can be applied in the bioeconomy. Such as utilizing remaining carbon dioxide (CO_2) from a biomethane upgrading plant for greenhouse crop farming by CO_2 enrichment (Journal Publication 2), proposing a novel bioreactor geometry, and performing a detailed CFD investigation to describe how the system's internal geometry affects the overall reactor's performance through mixing (Journal Publication 3, Journal Publication 4, and Conference Publication 1). CFD was also utilized to characterize different stirrers' performance (Journal Publication 5). A systems perspective was used to retrofit farm-opened anaerobic lagoons to self-sustainable covered lagoons and propose a new scalable two-stage anaerobic digester system that utilizes the kinetic energy from small wind turbines to mix the inside of the digester's contents (Journal Publication 6). Lastly, the thesis explores the concept of safe-by-design for biorefineries (Journal Publication 7), ensuring a holistic and sustainable approach throughout the entire bioeconomy process.

1.1. Paper summary

1.1.1. Journal publication 1

This work proposes a circular economy model for developing arid coastal regions. By combining the environmental know-how of two coastal desert regions on the American continent (the Atacama Desert in Chile and the Sonoran Desert in Mexico) with similar geographical characteristics a general model for a circular economy in stressed environmental conditions is developed. The proposed model includes the use of solar energy for water desalination and energy production, hydroponic farming, microalgae and seaweed for biofuels and biochemicals, anaerobic digestion for organic waste management and nutrient recovery, and hydrogels for irrigation. The model requires regional policies and governance to incentivize its adoption, and further studies are recommended to ensure its environmental, social, and economic sustainability before pilot testing.

1.1.2. Journal publication 2

This work proposes using unutilized carbon dioxide (CO_2) from biomethane plants for greenhouse crop farming. The study focuses on the Bruck an der Leitha (Austria) biogas plant and determines the number of hectares of greenhouses that can be enriched with CO_2. The optimal greenhouse designs for completely closed and partially opened greenhouses are calculated using two methodologies, a simplified and a detailed calculation. The study concludes that the optimal greenhouse areas for both methods agree and that using CO_2 for greenhouse crop farming can reduce biogas plant emissions. Additionally, the possibility of using the CO_2 by-product for algae farming is briefly mentioned.

1.1.3. Journal publication 3

This work investigates the use of air-lift reactors (ALRs) in biorefineries, focusing on the design and placement of draft tubes for better flow control and improved mass transfer. The study compares the flow characteristics of three different internal loop ALR geometries using CFD and finds that the squared single and double draft tube reactor had a higher downcomer velocity, higher turbulence kinetic energy, and lower loop circulation time than the other configurations. The study also shows that the ratio of the draft tube-vessel width and the distance between the draft tube and the fluid's surface affects the draft tube's loop circulation time. The paper concludes that further research is needed to determine the impact of different draft tube parameters on flow behavior in ALRs.

1.1.4. Journal publication 4

This work examines the hydrodynamic behavior of a double-stage internal loop air-lift bioreactor using CFD simulations. The study focused on analyzing the impact of different double-draft tube configurations on the hydrodynamics of the reactor. Ten different geometric configurations were investigated, with variations in draft tube placement, liquid height, the distance between draft tubes, and draft tube diameters. Results suggest that the placement of the draft tubes heavily influenced the hydrodynamic behavior of the reactor, with smaller distances between draft tubes and a funnel configuration leading to higher velocities. The study provides valuable insights into the optimal configurations of air-lift bioreactors, which could contribute to developing more efficient biorefining concepts. The findings can be used to forecast the most optimal configurations of airlift bioreactors and have significant value for developing more efficient bioreactor systems in the transition towards a sustainable bioeconomy.

1.1.5. Journal publication 5

This work emphasizes the importance of mechanical mixing in bioreactors for optimizing microorganism growth and productivity. The study utilizes CFD simulations with OpenFOAM® to predict the power number of various stirring devices in a lab-scale reactor. Experimental and simulation results of three different stirring devices were compared, and the study demonstrates the value of CFD models in optimizing bioreactor design and predicting their performance. The findings are relevant for industries seeking to optimize bioreactor design and enhance productivity through better mixing processes. While some simulation inaccuracies were observed, the study validates the usefulness of CFD models in bioreactor design optimization. Further research is recommended to identify methods for reconciling experimental and simulated values and minimizing any discrepancies.

1.1.6. Journal publication 6

In this work, a novel concept is proposed for a two-stage covered lagoon anaerobic digester that utilizes the wind's kinetic energy to power the stirring systems. The retrofit of opened anaerobic lagoons to covered lagoons is also proposed for reducing biogas emissions of livestock.

1.1.7. Journal publication 7

In this work, a safe-by-design framework for biorefineries is proposed. The framework emphasizes the integration of safety considerations from the conceptual design phase, ensuring secure and sustainable operations.

1.1.8. Conference publication 1

This work uses CFD to compare the hydrodynamics of internal loop air lift bioreactors with different internal configurations. The research integrates an in-house Lagrangian particles coupling utility into an Eulerian solver to evaluate the residence time distribution in each circulation loop. Each configuration showed its own strengths and weaknesses at different reactor heights, and the particle tracking simulations allowed for better flow visualization. The study highlights the potential for future research on multiphase bioreactors, such as comparing the behavior of multiphase systems between the Euler-Euler simulation coupled with Lagrangian particles and a three-phase simulation incorporating solid-liquid-gas phases. Additionally, incorporating heating jackets into the double and triple-stage internal loop air lift bioreactor configurations could be an interesting application. The findings provide valuable insights for optimizing and designing internal loop air lift bioreactors for various biological applications.

1.1.9. Conference poster 1

This work develops a circular economy model for desert coastal regions based on the water cycle. Solar energy is utilized to power a water desalination plant to get fresh water. This freshwater can be used for hydroponic farming in non-arable soil, such as Antofagasta, or irrigation water dosing with hydrogels in semi-arable soil, such as agricultural land in Sonora. Seawater is suitable for microalgae production in raceway ponds, while seaweed can be farmed in the ocean for biochemical production. Microalgae can be used for biofuel production, among other applications. The residue streams from agricultural systems, microalgae, and seaweed can be processed through anaerobic digestion to produce biogas, with the digestate providing nutrients for agriculture. Biogas can be upgraded into biomethane, with CO_2 as feed for the microalgae. At the same time, a combined heat and power (CHP) unit can produce electrical energy for the grid and heat for desalination, capturing the exhaust gas and purifying it, and feeding the CO_2 to the microalgae.

Recovered nutrients from the digestate can be added to the hydroponic system. Additionally, byproducts like glycerol from biofuel production can improve biogas yields in anaerobic digestion.

1.1.10. Conference poster 2

This work uses the Anaerobic Digestion Model Number 1 (ADM1) to determine the biogas yield in the co-digestion of nopal cladodes with cow manure, swine manure, and chicken manure. The nopal cladodes are mixed with each manure on a ratio of 3:1, and the chemical characteristics for each substrate were taken from the literature. The results showed that the combination of cow manure and nopal cladodes performs better than those of swine manure and nopal cladodes and chicken manure and nopal cladodes. The potential benefits of using nopal cladodes in biogas production are highlighted due to their endurance to drought and arid conditions provided by their crassulacean acid metabolism. Research has shown that accurate calibration of the ADM1 requires experimental data to determine the biochemical parameters of the mixtures at different phases of the anaerobic digestion process. Therefore, further research is necessary to achieve a complete stoichiometric characterization of the process.

1.1.11. Conference poster 3

This work uses CFD to simulate the flow of six different internal loop airlift bioreactor geometries with different interior configurations. The simulations were conducted using the open-source software OpenFOAM®, and the results show that varying design parameters can lead to optimal configurations that can lead to more efficient biorefinery concepts. It was found that splitting the draft tube enhances mixing on the upper part of the bioreactor, and the ratio of bioreactor diameter versus draft tube diameter affects the downcomer velocity.

1.1.12. Public report 1

In this report, a state-of-the-art review of anaerobic digestion and biorefinery system levels design focused on supply chain management, scalability, retrofitting, recovery of volatile fatty acids, nutrient recovery, and sustainability assessment methodologies for biorefineries.

1.1.13. Public report 2

In this report, a state-of-the-art review of reactor geometries and operating condition statuses was performed. Computational fluid dynamic simulations were utilized for several anaerobic digester and biorefinery systems. The modeled systems were continuously stirred tank reactor, plug flow digester, bubble column, and air lift reactor.

1.1.14. Public report 3

In this report, an open-source toolbox was disseminated to study bioreactor systems. The toolbox consists of a series of OpenFOAM® tutorials developed for bioreactors. In Chapter 1, the importance of bioreactor modeling is addressed. Chapter 2 is an introduction to the open-source software OpenFOAM®. Chapter 3 is a tutorial on power consumption estimation on CSTRs with CFD. Chapter 4 is a tutorial on multiphase mixing with CSTRs. Chapter 5 is an upscaling tutorial for pneumatic-driven anaerobic digesters or bubble columns. Chapter 6 is a tutorial on how to perform optimization of airlift reactors based on our previous research.

1.2. Aim of the work

The aim of the thesis is to explore and develop sustainable solutions for various environmental challenges by utilizing circular economy models and optimizing bioreactor designs. The thesis includes seven journal publications, one conference publication, three posters, and three reports that cover a range of topics, such as circular economy models for arid coastal regions, the use of unutilized carbon dioxide for greenhouse crop farming, the hydrodynamic behavior of air-lift bioreactors, the importance of mechanical mixing in bioreactors, and a novel concept for a two-stage covered lagoon anaerobic digester. The thesis aims to provide valuable insights for developing more sustainable solutions for various environmental challenges, such as reducing CO_2 emissions, water scarcity, and organic waste management. Furthermore, it introduces a safe-by-design framework, ensuring the integration of safety considerations within the scope of biorefineries and bioeconomy development.

Chapter 2. State-of-the-art

2.1. Circular economy

The circular economy represents a significant shift away from the current linear production systems. It is a new paradigm that requires a fresh perspective to achieve significant breakthroughs. Boardman and Sauser (2008) suggest that leveraging minor shifts in perspective is crucial to realizing the potential of the Circular Economy (CE). Pearce and Turner (1989) introduced the concept of CE in their book, highlighting the interdependence between the environment and the economy. There are several definitions of the CE, but two of the most cited are the following. CE can be defined “as an economic system that replaces the conventional concept of "end-of-life" with a focus on reducing, reusing, recycling, and recovering materials throughout the production, distribution, and consumption processes” (Kirchherr et al., 2017). This definition emphasizes the importance of reducing waste by effectively managing materials across their life cycle. Another widely cited definition, put forth by the Ellen MacArthur Foundation (2015), characterizes the CE as "a new economic model that is restorative or regenerative by design and focuses on resource-related challenges for economies and businesses." In this context, the CE is centered around designing a life cycle that eliminates waste by using it as a feedstock or recirculating it.

According to Skawińska and Zalewski (2018), CE can be utilized as an effective management model to achieve sustainable development. This model can be applied in various ways, such as establishing and enforcing environmental regulations, developing a circular resource management system, promoting stakeholder cooperation in a collaborative sharing economy, and building social capital.

The main objective of the CE is to minimize waste by adopting a carefully planned life cycle approach that involves using waste streams as feedstock and recycling waste within the system (Balachandran et al., 2021). The European Union has emphasized the importance of achieving circularity through its Circular Economy Action Plan (European Commission, 2020), which prioritizes the transition towards a circular economy.

2.2. Circular bioeconomy

The bioeconomy refers to an economy where the fundamental constituents for materials, chemicals, and energy production are obtained from renewable biological resources (McCormick and Kautto, 2013). The European Bioeconomy Action Plan (European Commission, 2019) defines the bioeconomy as a comprehensive framework encompassing various sectors and systems reliant on biological resources, including animals, plants, micro-organisms, and derived biomass, along with their associated functions and principles. The bioeconomy encompasses the utilization of land and marine ecosystems and their services, primary production sectors such as agriculture, forestry, fisheries, and aquaculture, as well as economic and industrial sectors that leverage biological resources and processes to generate food, feed, bio-based products, energy, and services (European Commission, 2019).

The circular bioeconomy can be seen as the intersection or merging point between the circular economy and the bioeconomy (Tan and Lamers, 2021). The concept of circular bioeconomy represents the integration of the objectives of the circular economy and the bioeconomy, encompassing different levels of focus on biotechnology (Kershaw et al., 2021).

The successful implementation of the bioeconomy requires collaboration between governments, the private sector, and academia. Academia and the private sector must work together to advance lab-scale and pilot-scale prototypes to an industrial scale. Governments can incentivize the private sector to invest in biorefinery systems by establishing appropriate regulations (Philp, 2018). Institutions play a crucial role in driving technology development for the bioeconomy (Cabrera-González et al., 2022). To enable the development of the bioeconomy, it is essential to invest in research and infrastructure and bridge the gap between demonstration and industrialization by promoting the development of large-scale biorefineries (Global Bioeconomy Summit, 2020). The bioenergy industry is expected to play a crucial role in realizing a biobased economy by providing the necessary industrial infrastructure for transitioning towards biorefineries (Van Ree, 2017). Recognizing the potential of co-producing bioenergy and biomaterials in biorefineries, the International Renewable Energy Agency has emphasized its significance in reducing carbon emissions across various industrial processes while meeting the increasing demand for sustainable production (IRENA, 2020). Biorefining is considered the optimal solution to achieve large-scale sustainable utilization of biomass in the bioeconomy, which entails addressing the challenges of technology development and scaling up biorefinery operations by adopting best practices (IEA Bioenergy, 2015).

Within the context of the circular bioeconomy, biorefineries, including their essential components such as bioreactors, play a vital role as they provide the necessary infrastructure for the sustainable utilization of biomass, production of bioenergy and biomaterials, thus contributing to the circularity of resources.

2.3. Biorefineries

Biorefineries offer potential pathways for fabricating polymers, organic chemicals, fuels, and electricity from biomass produced with complex processing technologies (Maity, 2015). The biorefinery concept, with its cascading approach of utilizing biomass feedstocks, has emerged as a critical component of the bioeconomy, offering the production of multiple valuable products such as proteins for human food and feed, biofuels, biochemicals, and bioplastics, while seamlessly integrating with established biotechnologies like anaerobic digestion for the generation of bioenergy and fertilizer (Vance et al., 2022). Biorefineries have different classifications depending on the feedstock they process, the processes taking place, and the produced products.

Under the first classification, there are four generations. The first generation includes agricultural crops, the second generation comprises residues, agroindustry residues, and non-edible crops, the third generation includes algae, and the fourth generation includes genetically modified microalgae (Moncada et al., 2014). The International Energy Agency task 42 workgroup proposed the second classification, which consists of a systematic classification system that describes different biorefineries depending on their platforms, products, feedstocks, and processes (Cherubini et al., 2009). The last classification is according to the products and by-products they produce, and they can be classified as energy-based biorefineries (biofuel, biopower, bioheat/cold, and biogas), product-based biorefineries (chemical-based and material-based), and flexible biorefineries, which can change their production from food ingredients to non-food products based on market prices and demand (Moncada et al., 2015; Van Ree, 2017). Different families of products should be integrated with first, second, and third-generation feedstocks to have a flexible biorefinery.

In Europe, there are currently 224 biorefineries operating, with different feedstocks and product types. These include 63 biorefineries running on sugar and starch for bioethanol and other chemicals, 118 biorefineries running on oil and fat feedstocks for biodiesel and oleo-chemistry, 25 biorefineries running on wood, five biorefineries running on lignocellulose, and 13 biorefineries running on biowaste (BBIC, 2017). Several pilot plants have also been tested, such as green biorefinery, lignocellulosic biorefinery based on beech wood, lignocellulose feedstock biorefinery, and microalgae biorefinery (Ecker et al., 2012; Kamm et al., 2010; Laure et al., 2014; Michels and Wagemann, 2010; Nurra et al., 2014).

Biorefinery processes involve pre-treatment, fermentation, and downstream processing, and their efficiency depends on factors such as reaction kinetics, metabolic state, cell physiology, reactor design, instrumentation, control, and separation processes (Cabrera-González et al., 2021).

Bioreactors, also known as fermenters, are crucial in biorefinery operations. They provide a controllable environment for transforming low-value substrates into high-value products using living cells or enzymes (Singh et al., 2014). The main types of bioreactors are continuously stirred tank bioreactors, bubble column bioreactors, airlift bioreactors, fluidized bed bioreactors, packed bed bioreactors, and photobioreactors (Ramonet and Harasek, 2021).

CSTRs are widely used in biorefineries to make liquid concentrations uniform, transfer heat, disperse gas bubbles, and suspend particles and cells in the fluid (Schügerl, 1990). Photobioreactors utilize light energy for photosynthetic processes and can be categorized as open or closed systems (Ho et al., 2011).

Mixing systems in bioreactors can be mechanical or hydraulic (pneumatic). Mechanical mixing employs impellers driven by electric motors, and the power consumption is determined by the dimensionless power number (Ramonet and Harasek, 2021). Different types of impellers, such as turbines and paddles, are used for mechanical mixing in bioreactors (Ramonet and Harasek, 2021).

Among the novel bioreactors, the air lift bioreactor provides low shear forces during mixing, low energy consumption, and adequate heat and mass transfer, as mentioned in **Journal Publication 4**. ILALRs belong to the category of modified bubble column reactors, characterized by a baffle or draft tube that serves to split the internal structure. The ALR is structured into four hydrodynamic sections, including the riser, gas separation, downcomer, and bottom clearance while employing a pressure gradient generated by the average density between the riser and the downcomer as a pneumatic mixing strategy (**Conference Publication 1**). The four hydrodynamic zones of the ILALR can be seen in Figure 1.

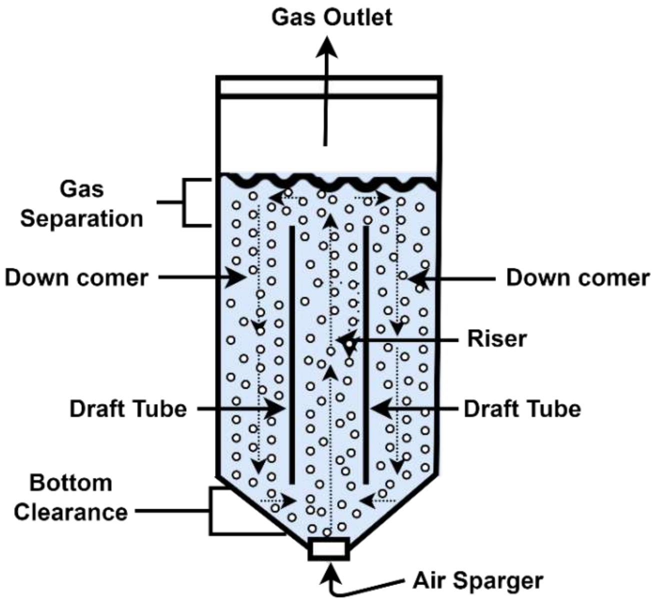


Figure 1. Schematic of Internal Loop Air Lift Reactor. Adopted from **Conference Publication 1.**

During the state-of-the-art review conducted for bioreactors in **Public Report 2**, a relatively unexplored geometry known as the multi-stage internal loop air lift reactor was discovered. It was first proposed by Blenke (1979), where it was found that when dividing the draft tube section into two or three sections, the mixing was enhanced. As a result, multi-stage concentric draft tube geometries were developed, aiming to improve performance. Blenke's divided draft tubes demonstrated significant reductions in mixing time, achieving up to 80 % reduction for double draft tubes and up to 87.50 % for triple draft tubes (Blenke, 1979). In a separate study, Siegel and Merchuk (1988) conducted experimental investigations on an internal loop split ALR by modifying the volume of the gas-liquid separator, a crucial factor influencing the reactor's mass transfer coefficient.

Several experimental studies have investigated the characteristics and behavior of multi-stage internal loop ALRs. Li and Qi (2014) focused on examining the flow patterns and hydrodynamics of such reactors. Li et al. (2018) studied the specifics of bubbles and the hydrodynamics within a two-stage internal loop ALR involving three phases. In a separate study by Tao et al. (2020), the emphasis was placed on hydrodynamics and mass transfer in a three-stage ILALR. Notably, this research highlighted the differences between gas-liquid bubbly flow and gas-liquid-solid slurry flow, emphasizing the significant implications of these distinctions for the reactor's performance and efficiency.

Regarding simulations with CFD, the only other authors who explored the multistage ILALR with CFD were Shi et al. (2021). In their study, Shi et al. (2021) investigated the effect of a contraction and expansion vane between the draft tubes.

In conclusion, biorefineries and bioreactors offer promising prospects for producing valuable products from biomass. The classification, processes, and design of biorefineries and bioreactors are critical in optimizing bioprocesses and achieving efficient conversion. The integration of already existing industrial infrastructure is explored in the following section.

A more detailed state-of-the-art on Biorefineries can be consulted in Chapter 2, “Biorefineries” of the appended report “CFD Optimization and Analysis of Existing AD and Biorefineries Report” (**Public Report 2**).

2.4. Integrating existing industrial infrastructure into biorefineries

Kromus et al. (2004) suggested incorporating anaerobic digesters into biorefineries as a valorization technique for generating lactic acid, amino acids, fibers, and energy within the green biorefinery framework. Continuing with the current emphasis on fostering a sustainable and circular bioeconomy, the convergence of biorefineries with existing biogas plants emerges as a groundbreaking technology with significant promise. The utilization of anaerobic digesters is a fundamental aspect of biorefineries (Sawatdeenarunat et al., 2016), serving as one of the final steps in the process of product valorization (Hagman et al., 2018). However, the challenge of scaling up biorefineries is a crucial issue to be addressed to facilitate a successful transition toward the bioeconomy, and utilizing existing infrastructure is essential in achieving this goal (Hingsamer and Jungmeier, 2019).

Determining the suitability of existing industrial infrastructure for retrofitting into biorefineries depends on several factors, such as product type, feedstock, transformation processes, and the platforms used (Cherubini et al., 2009). This classification system allows for the integration of biorefineries into these facilities. Biorefineries and existing industrial infrastructure share common features, and the combination of feedstocks and platforms is more critical than the combination of platforms and processes to facilitate integration (Jungmeier and Buchsbaum, 2014).

Utilizing the existing infrastructure of petroleum refineries can present a technically and economically feasible approach for the large-scale advancement of biobased biorefineries (Kumar and Verma, 2021). Additionally, IEA Bioenergy (2015) suggests that integrating biogas systems with other compatible processes, such as aquaculture, alcohol, or biorefinery systems, is another feasible combination.

In the field of biorefineries, the development of novel technologies is vital to ensure higher added-value production and stimulate the export of sustainable products and technologies, thereby increasing competitiveness (Hingsamer and Jungmeier, 2019).

By retrofitting existing industrial infrastructure systems into biorefineries, the principles of the circular economy are embraced through the reuse of facilities, resulting in minimized capital investments needed for establishing a biorefinery. Within this integrated framework, anaerobic digestion plays a crucial role in processing the organic residues and by-products generated by biorefineries. This biomass valorization cascading approach prioritizes the extraction of high-value compounds for pharmaceutical applications, followed by their utilization in food and feed production and, subsequently, in the production of bulk chemicals. Finally, anaerobic digestion is employed to generate bioenergy from the remaining biomass, completing the sustainable utilization cycle.

2.5. Anaerobic digestion

Anaerobic digestion (AD) is a widely used technology for treating organic waste, particularly in the context of biogas production. In AD, microorganisms break down organic matter in the absence of oxygen, producing biogas, mainly composed of methane and carbon dioxide.

A biogas facility utilizes biological microorganisms to convert plant and animal-based materials into methane, carbon dioxide, and other gases through anaerobic digestion (Sasse, 1988). The resulting biogas can be utilized to produce electricity and heat through a CHP unit or upgraded into biomethane, serving as a renewable natural gas (Laing et al., 2020).

According to the European Biogas Association (EBA) statistical report of 2020, Europe had 18,943 biogas plants by the end of 2019, of which 725 were biomethane plants (EBA, 2021). The distribution of biomethane plants in Europe was concentrated mainly in Germany, France, the United Kingdom, Sweden, the Netherlands, Denmark, and Switzerland, accounting for 90 % of the total, while the remaining 10 % were located in other European countries (EBA, 2021). Figure 2 shows the distribution of biogas plants in Europe per country.

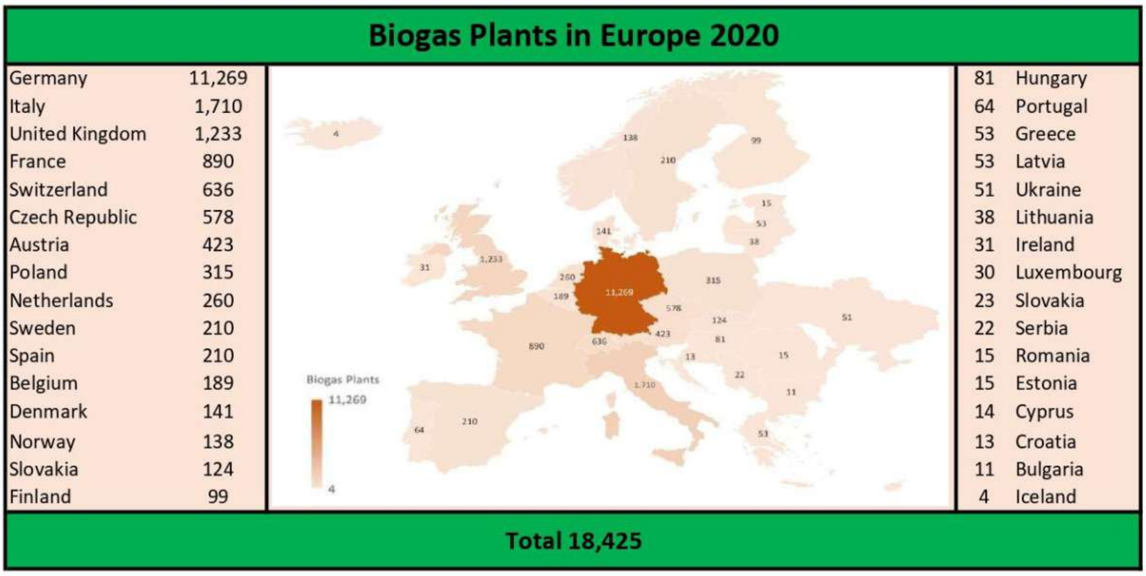


Figure 2. Biogas Plants in Europe 2020. Adopted from **Public Report 2**.

On a global scale, in 2019, there were 606 biogas upgrading plants worldwide, and Europe alone had 606 installed biomethane plants, as reported by the IEA Bioenergy Task 37 (2019). The predominant technologies used for biogas upgrading included water scrubbing, membrane separation, chemical scrubbing, and pressure swing adsorption (EBA, 2021; IEA Bioenergy Task 37, 2019).

The number of newly installed biomethane plants has shown a consistent increase over the years, with membrane separation technologies gaining popularity. This information is supported by data from the EBA (2021), which indicates a 16 % overall growth in the number of biomethane plants. Figure 19 of the appended **Public Report 2** provides insights into the distribution of biogas upgrading technologies across various European countries (EBA, 2021).

AD systems consist of different components, including feedstock pre-treatment, digester vessels, mixing systems, and control and monitoring systems. The choice of feedstock and its pre-treatment significantly influence the performance and efficiency of AD. Various pre-treatment methods, such as thermal, mechanical, and chemical processes, can enhance the digestibility of feedstock and increase biogas production (Carlsson et al., 2012; Krishna and Kalamdhad, 2014). Substrate characteristics, such as volatile solids content, moisture content, and particle size, play a crucial role in determining the performance of the AD process (Mshandete et al., 2006; Zamri et al., 2021).

Digester vessels are designed to provide optimal conditions for microbial activity. Different types of digester configurations, such as CSTRs, plug flow digesters, and covered lagoons, have their own advantages and disadvantages (Ramonet and Harasek, 2021). The selection of the digester configuration depends on factors like substrate characteristics, process stability, and specific requirements of the application.

Adequate mixing is crucial for maintaining a homogeneous environment and maximizing biogas production. Mixing modes can be continuous or intermittent and categorized as mechanical, hydraulic, or pneumatic (Mao et al., 2019). The mixing process's effectiveness depends on various factors associated with the rheology of the substrate, the vessel's design (including size and shape), the characteristics of the mixers (including quantity, placement, and orientation), and the operational procedure employed. These parameters encompass aspects such as the method of substrate feeding (continuous or intermittent), the temperature of the bulk liquid, the velocity of mixing, and whether the mixing is conducted continuously or intermittently (Conti et al., 2019). While mechanical mixing has been extensively studied, gas mixing remains poorly understood. The uniformity index and relative occupancy concepts offer improved analysis of mixing efficiency (Dapelo and Bridgeman, 2020).

The energy consumption of AD systems depends on various parameters, including substrate rheology, digester and mixer design, and operational procedures, such as mixing mode and time (Singh et al., 2019). Power input per unit digester volume increases logarithmically for scale-up digesters (Dapelo and Bridgeman, 2020; Wu and Chen, 2008). Maintenance and periodic cleaning of digesters are essential to prevent sedimentation and ensure optimal performance (Ramonet and Harasek, 2021).

Safety guidelines, such as the TOP (Technical, Organizational, and Personal) protective measures principle, should be followed to ensure the safety of biogas plants (Bontempo et al., 2016). Monitoring and control systems are crucial for maintaining process parameters within the desired range. Flow, temperature, pH, and gas composition sensors are commonly used for process monitoring.

Co-digestion, the mixing of different waste or feedstock for AD, offers several advantages, including efficient use of equipment, cost-sharing, and improved methane yield (AgSTAR, 2011). The choice of co-substrates depends on their chemical characteristics, such as pH, total solids, volatile solids, and nutrient content. **Conference Poster 2** explores the co-digestion of farm manures (cow, swine, and chicken) with nopal cladodes from prickly pear cactus, which, thanks to its crassulacean acid metabolism, requires less water. Danzì et al. (2020) explored the feasibility and possible location of a biogas plant operating on prickly pear cactus in Italy.

In summary, AD is a versatile and efficient technology for organic waste treatment and biogas production. Proper feedstock pre-treatment, selection of digester configuration, adequate mixing, energy optimization, maintenance, and safety measures are critical for successful AD operation. The following section explores the utilization of modeling and simulation for bioreactor design and optimization.

More details on AD can be consulted in Chapter 3, “Anaerobic Digestion” of the appended report “CFD Optimization and Analysis of Existing AD and Biorefineries Report” (**Public Report 2**).

2.6. Modeling and simulation

The use of modeling and simulation plays a critical role in optimizing bioreactor design and finding the most effective retrofit solutions for anaerobic digesters. By iteratively simulating different operating conditions using a variety of input parameters (such as inlet flow, temperature, viscosity, mixing rate, and pH) and using the results as constraints for the integration of design experiments, engineers can develop the most cost-effective and yield-efficient bioreactor designs. Modeling and simulation are powerful tools for solving complex engineering problems where analytical solutions are unavailable (Zavalani and Kaçani, 2012). They can significantly enhance the development of chemical engineering systems (Chinda et al., 2019).

The term simulation refers to the use of mathematical equations, such as linear or non-linear algebraic equations, inequalities, and differential equations, to represent the characteristics or behavior of a real system (Verma, 2014). Since analytical solutions are often difficult to obtain, numerical methods are typically used for solving the equations (Verma, 2014). In engineering, simulation involves creating an idealized, computationally-manageable model of a "real" system to represent its dynamic behavior through software simulation (Zavalani and Kaçani, 2012).

The primary purpose of simulations is to estimate the behavior of a system under specific conditions. Simulation techniques are widely employed to design products and systems, analyze risks, test prototypes, perform predictive maintenance, and evaluate existing systems (Larman and Basili, 2003; Szczerbicki and White, 2010; Tahera et al., 2017; White, 1995; Zurcher and Randell, 1968).

Moving forward, we will now investigate the field of CFD. CFD is a powerful numerical simulation technique used to analyze and predict fluid flows based on fluid mechanics principles. CFD simulation allows for the detailed visualization and analysis of flow patterns, velocity distributions, pressure gradients, and other flow properties by solving a set of mathematical equations discretized and solved numerically using advanced computer algorithms. This technique has found significant applications in the bioeconomy sector, particularly in biorefinery systems' design, optimization, and retrofitting, including bioreactors. By simulating various scenarios and configurations, CFD provides valuable insights that help optimize bioreactor designs, improve performance, and make informed decisions regarding process parameters.

2.7. Computational fluid dynamics

Computational Fluid Dynamics (CFD) is a numerical simulation technique used to analyze and predict fluid flow behavior based on fluid mechanics laws. It involves solving a set of mathematical equations, known as the conservation laws or Navier-Stokes equations, which describe the principles of mass, momentum, and energy conservation. Additionally, equations for turbulence and other relevant physical phenomena are included to capture the complexities of real-world fluid flow. To perform the simulations, the equations are discretized and solved numerically using advanced computer algorithms. This allows for the detailed visualization and analysis of fluid flow patterns, velocity distributions, pressure gradients, and other flow properties.

CFD simulation is a novel technology that has gained recognition for its ability to numerically solve the conservation equations of momentum and mass and describe the mixing efficiency in various geometries (Zhendong et al., 2012). CFD simulation is a powerful method for describing the mixing efficiency in different process equipment, including reactors, heat exchangers, and centrifugal pumps, and it has been widely used in chemical and petrochemical processes, where it has achieved significant advancements (Quiroz-Pérez et al., 2019; Zhendong et al., 2012).

In the field of the bioeconomy, CFD is widely utilized to design, optimize, and retrofit biorefinery systems, particularly bioreactors. By simulating various scenarios and configurations, CFD provides engineers and scientists in the bioeconomy sector with valuable insights. These insights help optimize the design of bioreactors, improve their performance, and make informed decisions regarding process parameters, such as fluid flow patterns, mixing efficiency, heat transfer, and mass transfer. Essential parameters like local velocities, turbulence, pressure, concentration, shear rate-dependent viscosity effects, and local reaction rates are analyzed by time-resolved calculation of 3D flow fields inside anaerobic digesters and bioreactors to obtain an optimal reactor geometry (Balachandran et al., 2021). Furthermore, CFD is employed to establish the correlation between physical and biological characteristics in bioenergy systems, helping in the design of an ideal physical setting that enhances the biological processes (Wu, 2013). The mixing efficiencies for various digester configurations can be verified using CFD software before construction takes place (Meroney and Colorado, 2009).

While simulations can never perfectly replicate reality, the predictions must be sufficiently accurate to facilitate process improvement or design (Wartha et al., 2022). The accuracy of CFD simulations relies heavily on the quality of input data, including boundary conditions and physical properties of the materials involved. It is important to note that CFD models are simplifications of real-world complexities, and phenomena like turbulence or multiphase flows may require additional empirical correlations or assumptions. Additionally, the computational cost associated with CFD simulations can be significant, particularly for large-scale or complex systems that require high-performance computing resources. Validating CFD results against experimental data is essential to ensure the reliability and accuracy of the simulations. Despite these limitations, CFD remains a valuable tool in the bioeconomy for exploring and optimizing biorefinery systems, contributing to developing sustainable and efficient processes for bio-based products and renewable energy production.

Journal Publication 4 describes the mathematical models and governing equations utilized in the ALR studies in this thesis.

2.8. Designing safe biorefineries

Safety considerations have historically been given lower priority during the initial conceptual design phase of biorefineries, with the conventional approach being to design the biorefinery first and evaluate safety aspects at a later stage (López-Molina et al., 2020).

There are eight main safe-by-design strategies. The different design methods are the probabilistic risk-based design, deterministic (safety factor-based design), fail-safe design (or fail-secure design), active safe design, passive safe design, vandal-proof design, idiot-proof (or fool-proof) design, fault-tolerant design, and circular design (van Gelder et al., 2021).

To ensure the safety of biorefineries through the "safe by design" approach, various disciplines such as biotechnology, nanomaterials, and chemical engineering are utilized. These disciplines collaborate to implement comprehensive safety measures, addressing concerns such as the containment of microorganisms, prevention of cross-contamination in feedstocks, and other potential hazards. By integrating advanced technologies and employing rigorous protocols, biorefineries can effectively mitigate risks, safeguarding both the environment and the well-being of workers. The safe-by-design approach prioritizes proactive safety considerations throughout the entire conceptual design process, ensuring that potential safety issues are identified and addressed early on to establish secure and sustainable biorefinery operations.

Chapter 3: Problem Statement

The transition to a circular bioeconomy is essential for addressing the environmental challenges posed by global warming and achieving sustainability goals. This thesis aims to explore various applications of circular bioeconomy in chemical engineering, focusing on developing a circular economy model for arid coastal regions, investigating the potential use of unutilized carbon dioxide from biogas plants for greenhouse crop farming, studying mixing in bioreactors using CFD, analyzing the hydrodynamic behavior of air-lift bioreactors with a focus on draft tube design, proposing a novel concept for a two-stage covered lagoon anaerobic digester and provide a framework for designing biorefineries through the safe-by-design methodology. The objective is to provide insights that can advise the design and optimization of bioreactors, promote sustainability, and enhance productivity across various industries. By addressing these research areas, this thesis seeks to contribute to the advancement of the circular bioeconomy and support the transition to a more environmentally friendly future.

Chapter 4. Research Approach

The research approach in this thesis involves a combination of theoretical analysis, CFD simulations, and case studies. The overall goal is to explore and evaluate various applications of circular bioeconomy in chemical engineering.

The thesis begins with a theoretical analysis of the global climate change problem, highlighting the need for significant changes in current norms, practices, and technologies to achieve the targets set in the Paris Agreement. It also discusses the initiatives and strategies adopted by the European Union to promote sustainability, circular economy, and bioeconomy.

The thesis then introduces the AgRefine project, which focuses on developing advanced biorefinery technologies for the agri-bioeconomy industry. The project is organized into three work packages (WP1, WP2, and WP3), and this thesis specifically falls under WP2, which is focused on system-level design.

In the subsequent sections of the thesis, several studies are presented as journal publications, conference proceedings, and ongoing manuscripts. Each paper addresses a specific aspect of circular bioeconomy and chemical engineering, utilizing different research methods and approaches.

Journal Publication 1 proposes a circular economy model for developing arid coastal regions, combining the environmental knowledge of two coastal desert regions. The model includes various technologies such as solar energy for water desalination and energy production, hydroponic farming, microalgae and seaweed for biofuels and biochemicals, anaerobic digestion for organic waste management, and hydrogels for irrigation. The research approach here involves conceptual modeling and the development of a general model for circular economy in stressed environmental conditions.

Circular economy models are proof of the understanding that sustainability and resource efficiency are not one-size-fits-all solutions. Rather, they are inherently influenced by each region and country's unique characteristics and dynamics. In this regard, it becomes evident that circular economy models must be tailored to the specific context of their implementation, taking into account many factors, such as geographical, environmental, social, and political constraints.

Geographical factors, including climate, natural resources, and topography, shape a region's potential for circularity. For instance, arid coastal regions with water scarcity may require innovative water management and conservation approaches as part of their circular economy framework. Similarly, regions rich in renewable energy sources might focus on harnessing these resources to power circular processes.

Environmental considerations are crucial in designing circular economy models that minimize ecological impact and promote sustainable practices. Understanding the local ecosystem, biodiversity, and environmental vulnerabilities enables the identification of strategies that prioritize resource conservation, waste reduction, and the mitigation of adverse environmental externalities.

Social factors encompass the social fabric, cultural values, and the needs and aspirations of local communities. Successful circular economy models consider the social dimensions of sustainability, ensuring inclusivity, equitable distribution of benefits, and social cohesion. They aim to create opportunities for job creation, economic empowerment, and community engagement, aligning with the aspirations and well-being of the population.

Political factors, including policy frameworks and regulatory environments, profoundly influence the feasibility and effectiveness of circular economy models. Supportive policies, incentives, and regulations can drive the adoption of circular practices, facilitate stakeholder collaboration, and enable the necessary investments in infrastructure, technology, and research and development.

Thus, it becomes evident that circular economy models are not generic blueprints but rather context-specific and adaptive frameworks. By embracing the complexities of regional and national contexts and considering the interplay of geographical, environmental, social, and political constraints, we can pave the way for the successful implementation of circular economy strategies that maximize resource efficiency, promote sustainability, and foster a more resilient and prosperous future for all.

As an example of how to fit different circular bioeconomy applications in the framework of chemical engineering, the case of desert coastal regions is taken to integrate the various applications comprehensively and sustainably.

The following methodology was used to develop the circular economy model for desert coastal regions (**Journal Publication 1**). The problem is investigated on how the public perceives it and how it really is; based on these points, a new perspective is created. This new perspective is supported by evidence of the different applied technologies. The relative strengths of the new perspective and the implications for future research are discussed, as shown in Figure 3. The results from this process are shown in Figure 21.

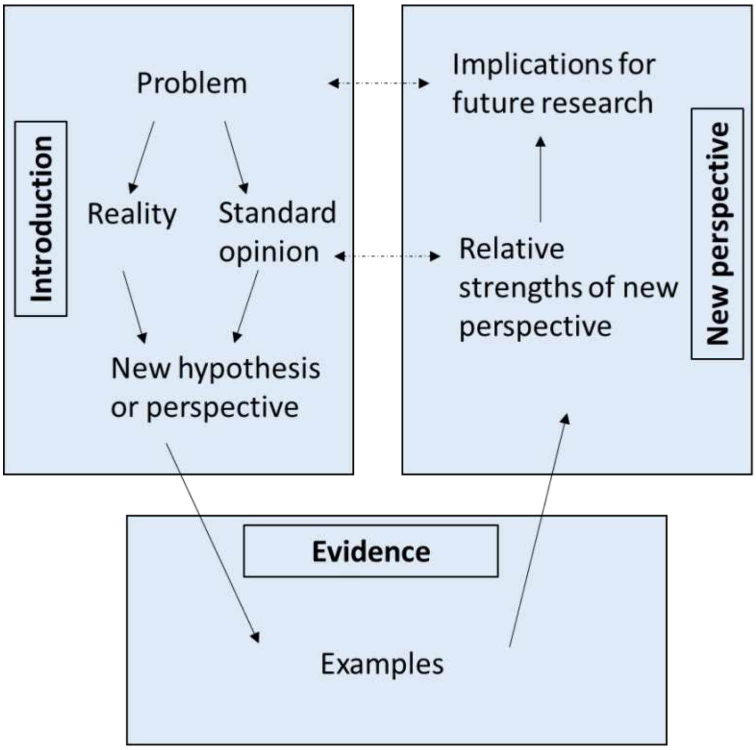


Figure 3. Methodology followed to develop the circular economy model.

The circular economy model proposed in **Journal Publication 1** was assessed by evaluating the attributes associated with its processes and products, i.e., biochemicals, biofuels, biogas, biogas upgrade, CHP, hydrogels, hydroponic, nutrient recovery, solar harvest, and water desalination. Each attribute was rated on a scale from 0 to 10, with a rating of zero indicating poor performance and a rating of ten indicating outstanding performance. The four attributes considered in the evaluation were technology readiness level, economic viability, ecological sustainability, and environmental risks. The technology readiness level assessed the readiness of the technology for deployment, while ecological sustainability evaluated its environmental impacts. Environmental risks refer to the potential irreversible environmental damage if the products or processes are not managed correctly, and economic viability considers the capital costs. The graph evaluating these parameters (Figure 20) is presented in the results section.

Journal Publication 2 explores the potential use of unutilized carbon dioxide (CO_2) from biogas plants for greenhouse crop farming. The study focuses on a specific biogas plant and calculates the optimal greenhouse designs for CO_2 enrichment. The research approach here involves data analysis, calculation, and comparison of greenhouse areas for different designs.

Once the circular economy model had been developed, the different technologies involved were studied for their optimization or other possible applications. An example of this is presented in **Journal Publication 2**, which examines a biogas plant near Vienna (approximately 40 km from the city center) as an example of efficient resource utilization in the circular bioeconomy.

The methodology employed in this study includes analyzing data, performing calculations, and comparing greenhouse areas across various designs. Two different methods were utilized for optimal greenhouse size calculation, a simplified and a detailed calculation.

For the simplified calculation, the monthly availability of sun hours was used to determine the number of hours suitable for utilizing CO_2 in greenhouse crop production. This calculation involves multiplying the daily daylight hours by the number of days in each month. The resulting number of hours, representing the CO_2 utilization period for greenhouse crop production, is then used to estimate the potential annual CO_2 utilization and the corresponding greenhouse area that can be enriched. Figure 4 shows the methodology followed in the simplified calculation to obtain the optimal greenhouse area for completely closed and partially opened greenhouses. The CO_2 consumption rates for completely closed and partially opened greenhouses are sourced from (Blom et al., 2002). The potential yearly CO_2 utilization is obtained by summing up the monthly values. Finally, the greenhouse area eligible for CO_2 enrichment is determined by dividing the annual available CO_2 from the biogas plant in Bruck an der Leitha by the potential yearly CO_2 utilization.

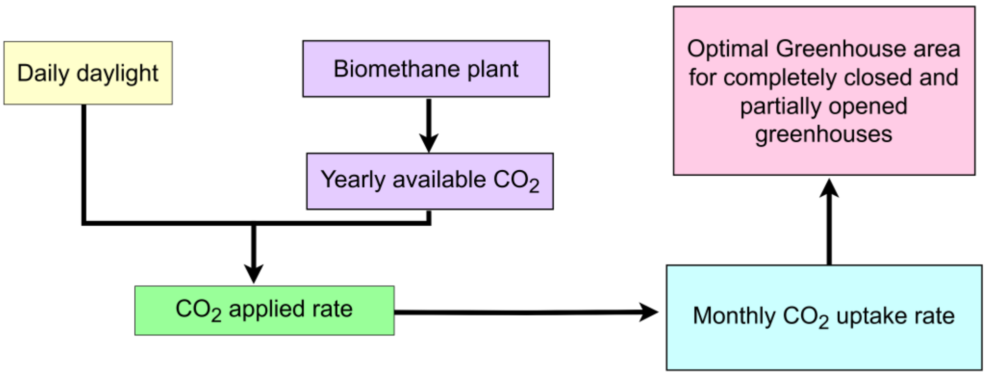


Figure 4. Schematic of the simplified calculation.

For the detailed calculation, the following methodology was used. First, it is considered that for a completely closed greenhouse, a fully-grown crop consumes carbon dioxide at a rate of 0.24 kg/h/100m^2 on a sunny day, and a small crop on a shady day has a CO_2 uptake rate of 0.12 kg/h/100m^2. The solar radiation and available daily daylight were utilized to extrapolate the monthly CO_2 uptake rate. By using the CO_2 uptake rate per 100 m^2 as a basis, this estimation determined the level of CO_2 enrichment in hectares for a fully enclosed greenhouse. The months of June and July, with their 16 hours of daylight, when CO_2 availability per hour is at its lowest, resulted in the smallest plantation areas.

Second, for a partially opened greenhouse, the same procedure with solar radiation was utilized. For a double polyethylene wall partially opened greenhouse, the minimum uptake rate was 25 kg/ha/h and the maximum 35 kg/ha/h. The minimum uptake rate for standard glass partially opened greenhouses was 50 kg/ha/h, and the maximum was 60 kg/ha/h. These values were taken from (Blom et al., 2002). The schematic of the methodology used is presented in Figure 5.

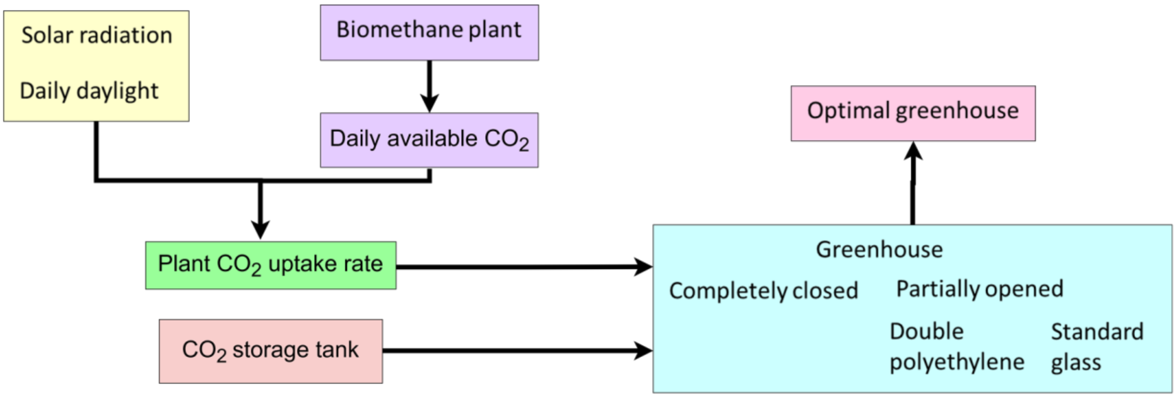


Figure 5. Schematic of detailed calculation. Extracted from (Ramonet et al., 2022b).

Microalgae are generally grown in raceway ponds or photobioreactors. Pneumatically stirred photobioreactors, which are a well-known technology, are commonly used. These systems often employ draft tubes to promote mixing. ALRs can be utilized for the production of biochemicals from seaweed, in addition to their application in microalgae cultivation. There are two main configurations of ALRs: external loop and internal loop. In the context of this thesis, the focus is on exploring the potential of internal loop ALRs.

In **Journal Publications 3, 4** and **Conference Publication 1**, the hydrodynamics of different ALR systems is explored with CFD, focusing on the design and placement of draft tubes. The methodology utilized for this section was first performing a state-of-the-art review to know which CFD model is well suited for predicting the global hydrodynamics of an air-liquid interphase. Then the accuracy of the discretization is evaluated with a mesh study.

Several measures were taken to ensure the reliability of the computational model utilized in the air lift reactor studies. The first step was to set up the model with the configurations employed in the literature. For this purpose, a two-fluid model was adopted, using an Euler-Euler approach for the simulations. The standard multiphaseEulerFoam solver was chosen for its suitability in simulating the behavior of gas bubbles within a liquid medium. The Euler-Euler model was coupled with the Large Eddy Simulation (LES) method to simulate the flow in the reactors accurately.

This multiphaseEulerFoam solver can effectively handle multiple compressible fluid phases, including at least one dispersed phase. In this case, air was employed as the dispersed phase, while water was the continuous phase. The mathematical models and governing equations mentioned here, are described in detail in **Journal Publication 4**. The Schiller-Naumman drag model, the NicenoKEqn sub-grid turbulence model, and the ContinuousGasKEqn sub-grid turbulence model were used. The NicenoKEqn model was specifically chosen to determine the turbulence of the fluid phase, as it is a one-equation sub-grid stress model suitable for capturing turbulence generated by bubbles. On the other hand, the ContinuousGasKEqn model was utilized to determine the turbulence of the gas phase and account for phase-inversion effects. The drag of each phase was solved using the Schiller-Neuman model, which calculates the drag forces acting on the particles. For this model, a single bubble size was considered, as it has been shown to provide reasonable predictions when comparing simulations to experimental results (McClure et al., 2017). A bubble diameter of 4.5 mm was chosen based on literature values ranging from 3 mm to 5 mm (van Baten et al., 2003). The diameter of water droplets was kept at the default value of 0.1 mm in the solver.

The second step to ensure the reliability of the computational calculations was performing a mesh convergency study. Numerous researchers recognize the significance of mesh refinement in mitigating rounding, iterative, and discretization errors (Almohammadi et al., 2013). A mesh convergence study is performed to evaluate the precision and reliability of CFD simulations by examining how the results are affected by variations in the mesh size. The purpose of this study is to identify the ideal mesh resolution needed to achieve accurate and consistent solutions.

Two mesh independency studies were performed. A vessel without any draft tubes with a conical bottom was utilized for both mesh studies. A diagonal line was plotted from the inlet to the outlet, and the air velocity magnitude was extracted from the first peak (same procedure as Figure 3 of **Journal Publication 4**) to calculate the grid convergence index.

As an example, the first mesh independency study is shown. The second is carefully described in **Journal Publication 4**. Five meshes (Figure 6) were selected from 23 thousand to 2.2 million cells for the first mesh independency study, with a grid refinement ratio of 1.5. The five meshes utilized for this mesh dependency study are shown in Figure 6. The air velocity magnitude for the five meshes is shown in Table 1.

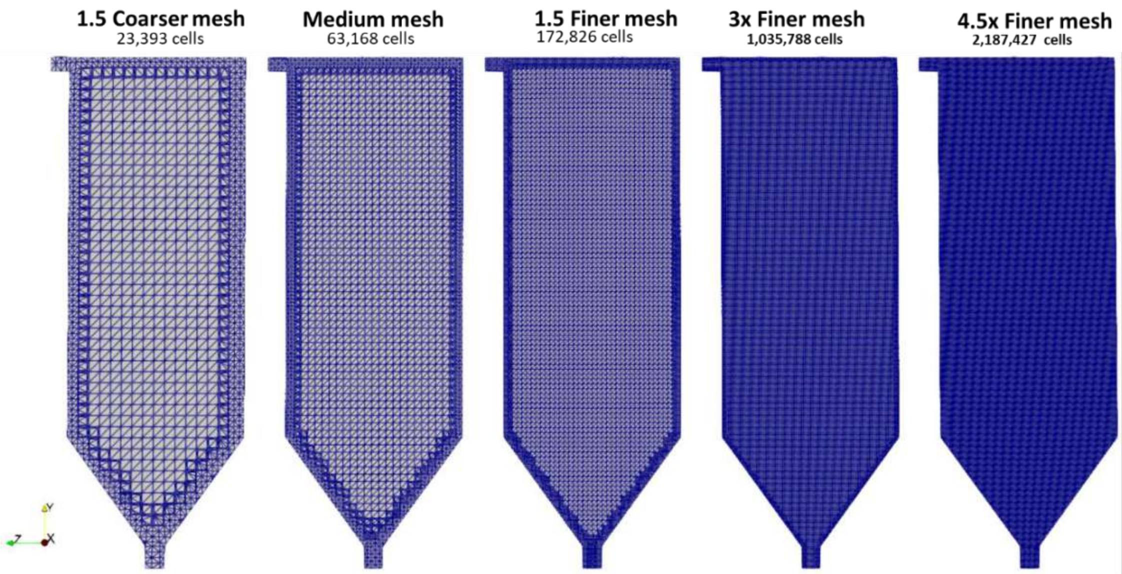


Figure 6. Meshes utilized in mesh study. Adopted from **Public Report 2**.

Table 1. Air velocity in different meshes. Adopted from **Public Report 2**.

Meshes	Air Velocity Magnitude (m/s)
M1-Coarser (1.5)	0.317141
M2-Reference	0.317388
M3-Finer (1.5)	0.317888
M4- Double Finer (3)	0.320667
M5-Triple Finer (4.5)	0.323351

The order of convergence is calculated with Equation 1. Three meshes are needed for this, the reference mesh (M2) as F_2, the coarser mesh (M1) as F_3, and the finer mesh (M3) as F_1. The finer meshes M4 and M5 were then utilized with the Richardson extrapolation (Richards, 1997) to verify the convergence between the calculated and simulated values. For Equation 1, r is the grid refinement ratio of 1.5.

$$p = \frac{\ln\left(\frac{F_3 - F_2}{F_2 - F_1}\right)}{ln(r)} \qquad \text{(Eq. 1)}$$

Once Equation 1 is resolved, we have that p equals -1.73929. The Richardson extrapolation (Richards, 1997), Equation 2, is then utilized to verify the convergence between the calculated values (extrapolated) and the ones extracted from the simulation. Then the grid convergency index (Equation 3) is used to extrapolate the air velocity magnitude for finer meshes.

$$F_0 = F_1 + \frac{F_1 - F_2}{r^p - 1} \qquad \text{(Eq. 2)}$$

$$GCI_{2,1} = \frac{\frac{F_2 - F_1}{F_1}}{r^p - 1} \qquad \text{(Eq. 3)}$$

Extrapolated values are obtained for mesh four (double finer) and mesh five (triple finer). In Table **2**, the extrapolated results are compared with the extracted ones, and then the error is obtained.

Table 2. Mesh convergence error.

Meshes	Extracted	Extrapolated	Error
M4- Double Finer	0.320667	0.319424	0.38 %
M5-Triple Finer	0.323351	0.320959	0.74 %

As a validation of the model, the squared geometry presented in **Journal Publication 3** was compared in the single draft tube configuration with inlet velocities of 0.01 and 0.02 m/s against the experimental data from the literature (Jia et al., 2007). In the results section, Figure 37 compares the simulated results with the ones from Jia et al. (2007).

Journal Publication 3 investigates the use of ALRs in biorefineries, focusing on the design and placement of draft tubes for better flow control and improved mass transfer. CFD simulations are utilized to compare the flow characteristics of different ALR geometries. The research approach here involves CFD simulations and analysis of the results.

In **Journal Publication 3**, the study investigated three different vessel geometries for ALRs and examined single and double draft tube configurations for each vessel. This resulted in a total of six different reactor configurations. The hydrodynamics of these reactor configurations were studied using CFD.

One of the geometries adopted in this study was a squared single draft tube configuration sourced from existing literature (Jia et al., 2007). To establish a comparative analysis, the draft tube was divided into two, with the separation distance between the draft tubes matching the distance between the inlet and the bottom of the lower draft tube. Another geometry examined was a cylindrical double draft tube configuration, also obtained from the literature (Shi et al., 2021). A counterpart configuration with a single draft tube was developed specifically for this study to facilitate the comparison. The third geometry comprised a cylindrical reactor with a coned transition from the inlet to the body. The cylindrical section of this geometry was derived from the second geometry.

The draft tubes (single and double configurations) in the third geometry have the same geometric characteristics as the ones in the second geometry. These selected geometries were considered representative shapes for the ALRs analyzed in this study. Figure 7 shows these reactor configurations.

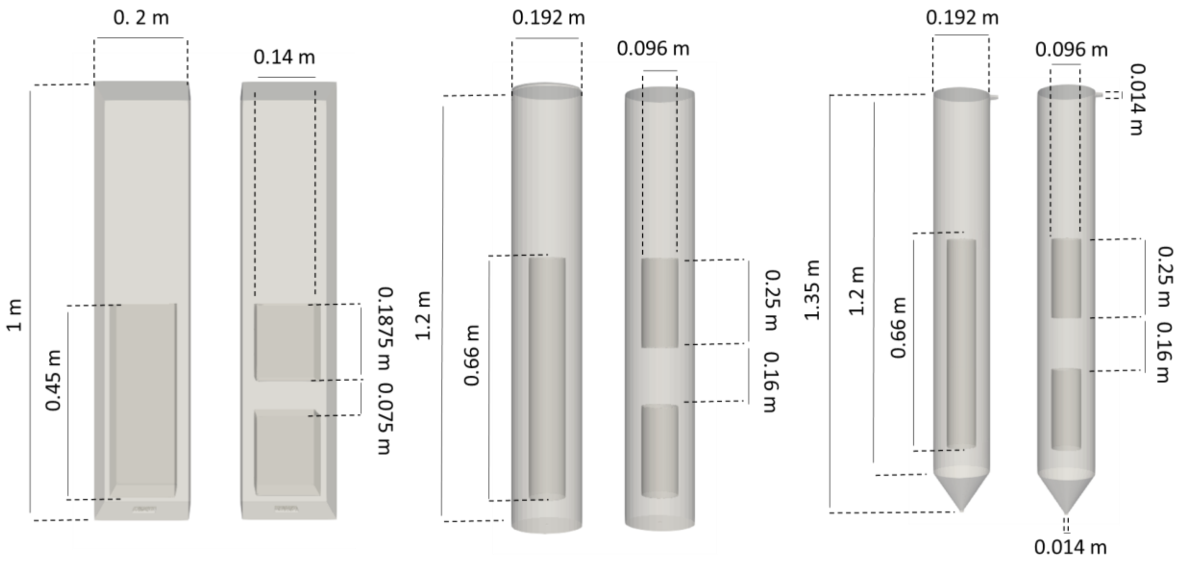


Figure 7. Geometries utilized for the study. Adopted from **Journal Publication 3**.

Various parameters were compared during the analysis, including turbulent kinetic energy in the fluid phase, fluid velocity along the Y-axis, pressure, and the circulation time of the draft tube loop. Among these parameters, the axial velocity in the downcomer section emerged as the most representative factor.

Building upon the previous research approach, **Journal Publication 4** explores into the hydrodynamic behavior of a double-stage internal loop air-lift bioreactor using CFD simulations. This study focuses on analyzing the impact of different double-draft tube configurations on reactor hydrodynamics. The research approach involves conducting CFD simulations, exploring various geometric configurations, and analyzing the results.

For **Journal Publication 4**, two of the previous geometries serve as input for further investigation. Figure 8 presents the geometries utilized in this study, highlighting their relevance to the research.

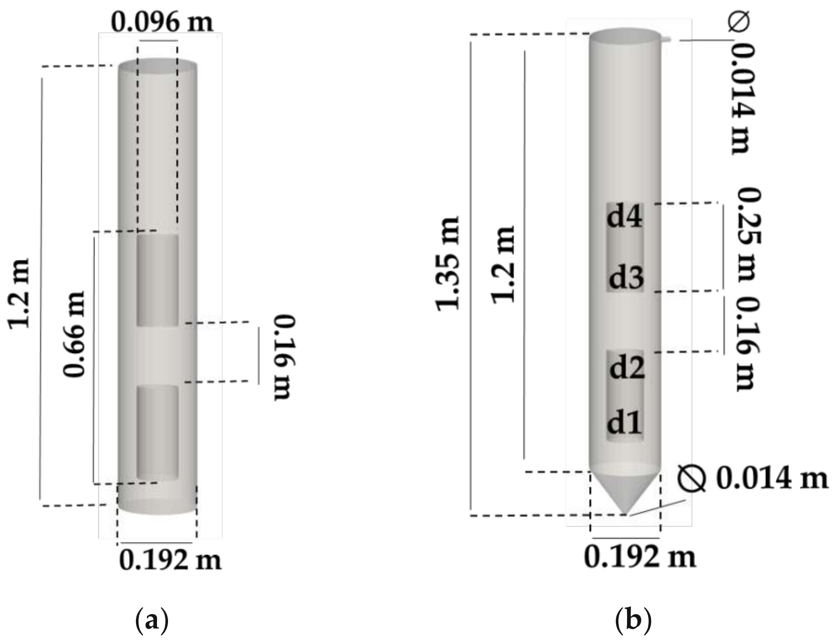


Figure 8. Geometries utilized in the study. Adopted from **Journal Publication 4**.

Ten distinct geometries are examined to explore the effects of different factors on the internal hydrodynamics of an ALR. Geometries one and three (Figure 9) were derived from **Journal Publication 3**, with modifications made to investigate the impact of varying liquid height, the distance between draft tubes, and acylindricity by altering the draft tube diameters on the internal hydrodynamics of an ALR. Geometry three is based on Shi et al. (2021), while geometry one is an adaptation that includes a coned bottom inspired by reactors used in wastewater treatment. Geometries four and five are unique because the top draft tube is displaced. In all other geometries, reducing the distance between draft tubes shifts the bottom draft tube's location. Figure 9 shows the ten geometries utilized in this study.

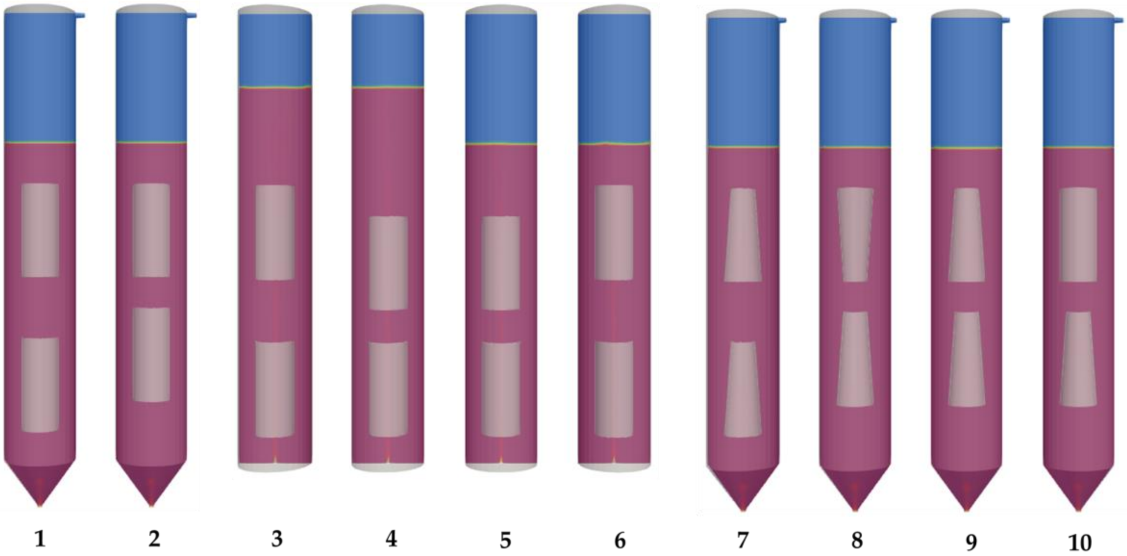


Figure 9. Ten geometries utilized in the study. Adopted from **Journal Publication 4**.

Calculating the loop circulation time involves extracting values from the riser and downcomer sections. Nine points were sampled on the riser (marked with a U in Figure 10), and another nine points were sampled on the downcomer (marked with a D in Figure 10). Using the extracted velocity values, the velocity was interpolated between each point until a loop was formed. A similar approach was reported in the literature, where the total circulation time was calculated by summing the ascending and descending times for a single draft tube geometry (Padial et al., 2000). For this study, the connection between the riser and the downcomer was also calculated by interpolating the velocity of the vector moving in this direction.

The "first draft tube" loop is determined by measuring the time it takes for a particle to follow a path from the inlet, rise to the top, descend until it reaches the end of the top draft tube, and then reintegrate into the flow, forming a complete loop as depicted by the blue arrows in Figure 10. Similarly, the "second draft tube" loop refers to the time it takes for a particle to travel from the inlet, ascend to the interphase section, descend to the bottom of the lower draft tube, and complete a loop, which is illustrated by the black arrows in Figure 10. This strategy is utilized to compare the residence time in each loop.

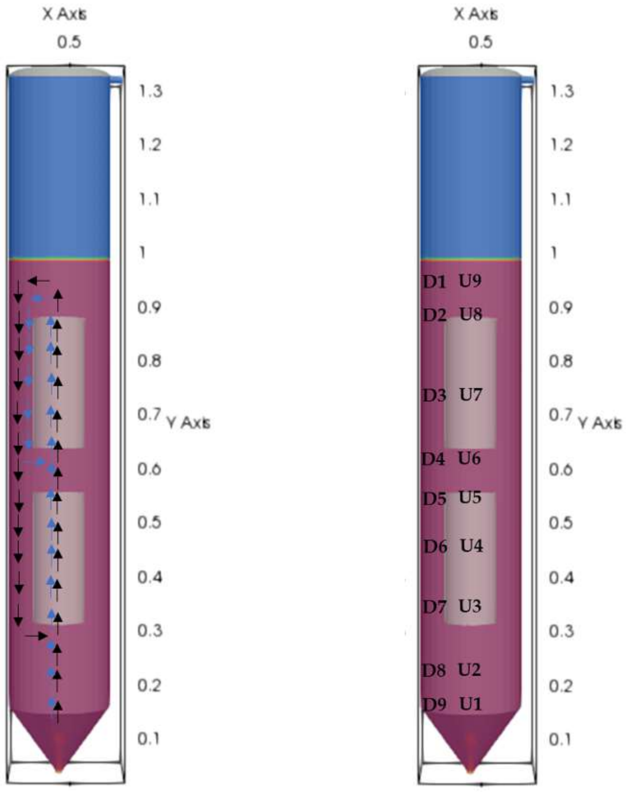


Figure 10. Circulation loop and sample points. Adopted from **Journal Publication 4**.

Continuing in the same line of research, **Conference Publication 1** utilizes CFD to compare the hydrodynamics of internal loop air-lift bioreactors with different internal configurations. The research approach integrates an in-house Lagrangian particles coupling utility into an Eulerian solver, enabling the evaluation of residence time distribution and flow visualization.

Building upon this approach, **Conference Publication 1** explores the concept of the conned bottom reactor. This publication focuses on investigating the global hydrodynamics of single, double, and triple draft tubes. To establish the reactor geometry, an airlift column reactor with an aspect ratio (height to diameter ratio) of approximately 10, including the inlet tube, was chosen based on Chisti and Young's findings (Chisti and Moo-Young, 1987). Figure 11 shows the three geometries utilized in this study; a total reactor height of 1.9 meters and a diameter of 0.196 meters were used. The liquid height was set to 1.55 meters for all cases, the bottom clearance (distance from the inlet to the bottom draft tube) was 0.256 meters, and the top clearance (distance from the top draft tube to the surface) was 0.472 meters. As shown in Figure 11, the draft tube section is 1 meter in length and 0.098 meters in diameter; the distance between draft tubes was 0.0875 meters.

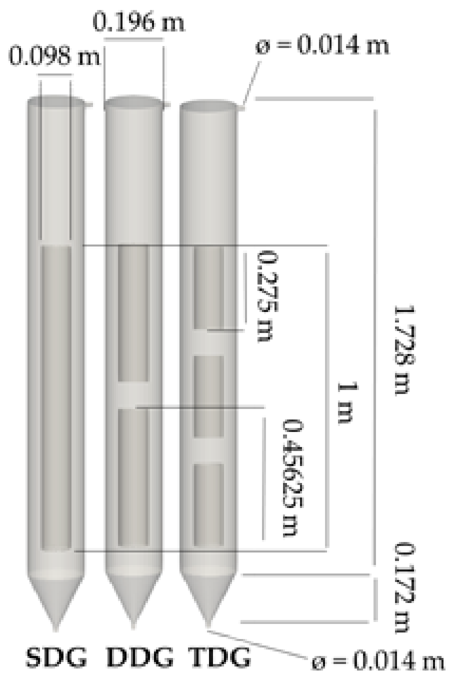


Figure 11. Single, double, and triple draft geometries. Adopted from **Conference Publication 1**.

To investigate how splitting the draft tube affects the ALR flow, 16 points were selected on the riser and downcomer to compare the axial velocities on both sections. Then five representative points were chosen on the downcomer at the bottom and above each draft tube to compare the turbulent kinetic energy, the fluid's velocity, and the pressure. These five points are shown in Figure 12.

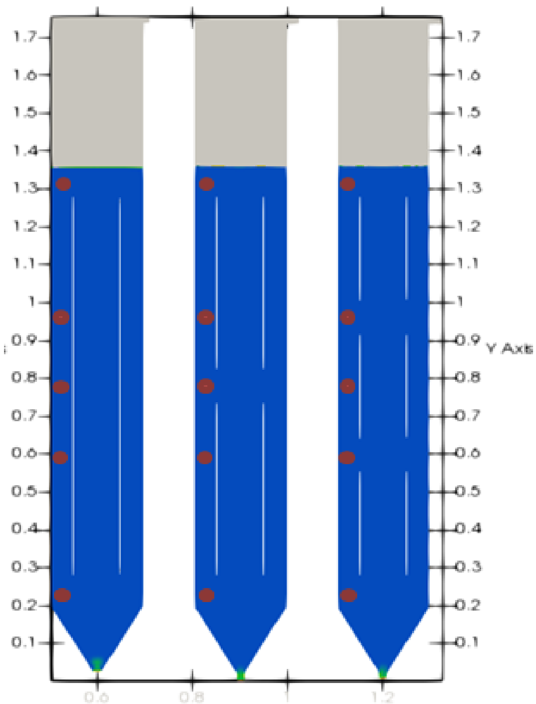


Figure 12. Probes for measuring. Adapted from (Ramonet et al., 2023).

An in-house Lagrangian particle utility called “Lagrangian plug-in for multiphaseEulerFoam,” developed by Bosenhofer (2022), was integrated into the multiphaseEulerFoam solver of OpenFOAM® version 9. This integration allowed for the coupling of Lagrangian particles with the continuous phase of an Euler-Euler simulation. By utilizing this utility, the residence time distribution in each draft tube could be evaluated, providing valuable insights into the flow and circulation loops within the three different geometries.

As mentioned above, CFD was utilized to evaluate these reactor geometries by evaluating the draft tubes' circulation time and the axial water velocity from the riser and downcomer sections. A two-fluid model was chosen to perform the CFD hydrodynamic calculations were resolved using the multiphaseEulerFoam solver, which is part of the open-source toolbox OpenFOAM® version 9. The solver is based on the Euler-Euler model (a type of two-fluid model) that employs the Lagrangian framework to track the movement of individual parcels.

Moving from the investigation of ALRs in the previous section, **Journal Publication 5** focuses on CSTRs. While ALRs are commonly used for microalgae cultivation, CSTRs are widely employed in the chemical, biochemical, and pharmaceutical industries as the preferred reactor type. In both cases, the hydrodynamic behavior and mixing characteristics are crucial in optimizing reactor performance. Therefore, the research approach transitions from studying ALR geometries to exploring the power number of various stirring devices in a lab-scale CSTR. By integrating CFD simulations, experimental data comparison, and model validation, **Journal Publication 5** aims to enhance our understanding of mechanical mixing and its impact on microorganism growth and productivity.

Journal Publication 5 focuses on the study of mixing in CSTRs, widely employed in the chemical, biochemical, and pharmaceutical industries as the preferred reactor type. These reactors rely on mechanical stirring mechanisms to ensure adequate mixing. The study emphasizes the significance of mechanical mixing in bioreactors to optimize microorganism growth and productivity. To achieve this, CFD simulations are conducted to predict the power number of various stirring devices in a lab-scale reactor. The research approach integrates CFD simulations, comparison with experimental data, and validation of the models.

In this study, experiments are conducted using three different stirrers in a 45-liter lab reactor with specific dimensions. Subsequently, CFD simulations are performed to compare the torque and power number associated with each stirrer. The reactor utilized in the experiments has a height of 65 cm and a radius of 15 cm. It is equipped with four baffles measuring 24 cm in height, 4.5 cm in width, and 0.6 cm in thickness. These baffles are connected at the bottom by a ring baffle with an inner radius of 8.4 cm, a height of 3.3 cm, and a thickness of 1.2 cm. The mechanical agitation in the reactor is controlled by a laboratory stirrer (IKA EUROSTAR 200 Control), which also serves as a torque measurement device.

The liquid height in the reactor was set to 42 cm, equivalent to 30 liters. In the computational domain (shown in Figure 13), the height of the reactor matched the liquid's height. The experimental setup and the CFD domain are depicted in Figure 13.

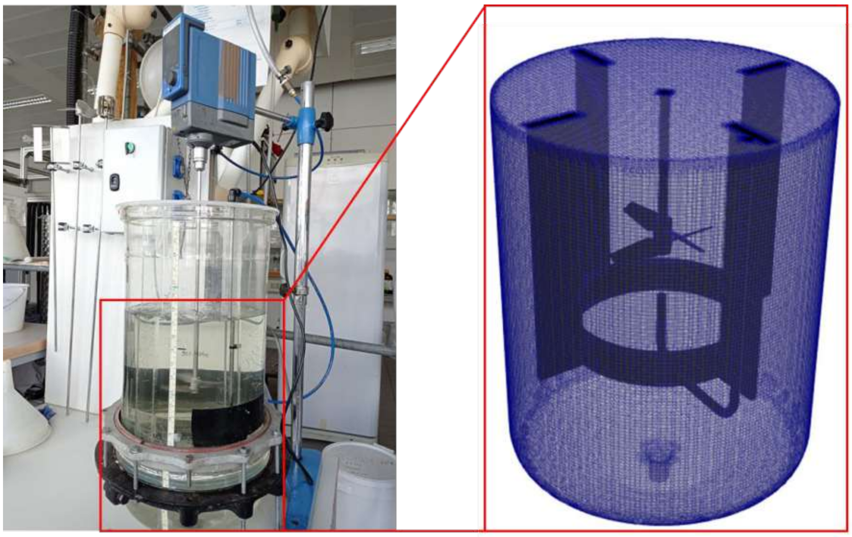


Figure 13. Experimental setup and computational domain. Extracted from **Journal Publication 5**.

The study used three types of stirrers: pitched blade, cage, and paddle. The stirrers are illustrated in Figure 14. The velocity was gradually increased during the experiments until unstable vibrations prevented torque measurement. Torque measurements were recorded for each stirrer type within specific RPM ranges: 550 to 1300 RPM for stirrer 1, 400 to 950 RPM for stirrer 2, and 130 to 325 RPM for stirrer 3.

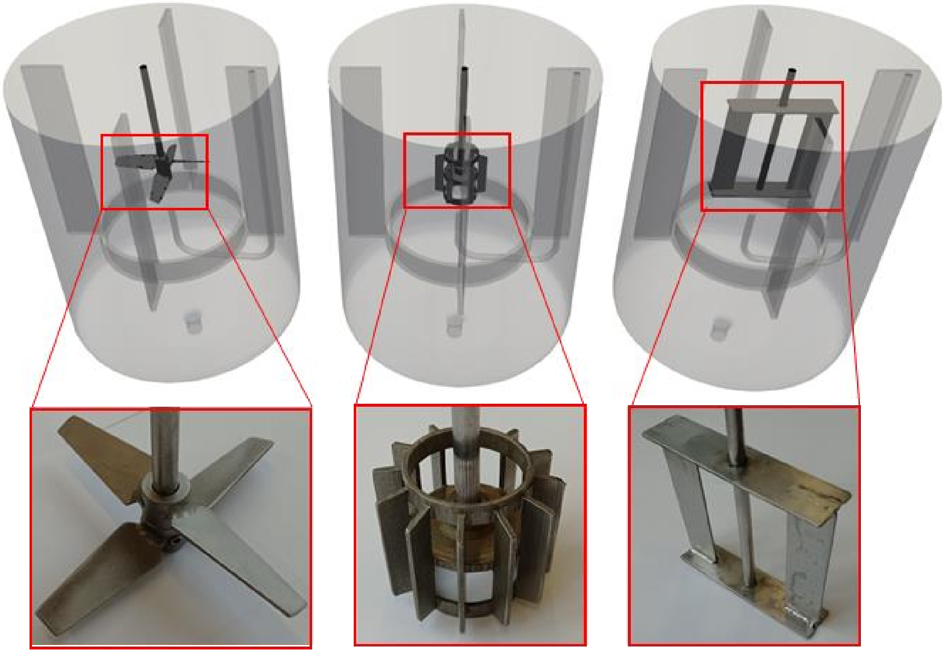


Figure 14. Comparison of Computational Geometries and Real Stirrers in Stirred Tank Reactors.

In this study, OpenFOAM® version 8 was employed using the single-phase SimpleFOAM solver. The SimpleFOAM solver utilizes the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm to solve for steady-state, incompressible, turbulent flow. The simulations focused on modeling the behavior of water as a single-phase fluid. The simulations achieved a residual convergence of approximately $1x10^{-6}$, with an average of around 520 iterations needed to reach this convergence, ensuring a smooth velocity field and reliability of the computational model utilized for the air lift reactor studies.

The Multiple Reference Frame (MRF) method was employed to simulate impeller rotation in the mixing systems. The MRF method is widely recognized as suitable for modeling stirred reactors and capturing flow and mixing generated by impellers (Ding et al., 2010). Accurate determination of the stationary and moving areas within the MRF method is crucial for obtaining precise results in terms of mixing performance (Foukrach et al., 2020). One of the advantages of the MRF approach is its relatively low computational time. It involves dividing the computational domain into two regions: a rotating cylindrical volume that encloses the impeller and a stationary outer volume encompassing the rest of the tank (Foukrach et al., 2020).

To obtain digital representations of the stirrers, stirrers 1 and 3 were fully digitized in terms of their geometries, while stirrer 2 had its number of blades reduced by half to six. Figure 13 illustrates the experimental setup with three reactors, including baffles and internal components, each equipped with one stirrer. The number of cells for each geometry is presented in the result section in **Journal Publication 5**. Mesh generation was achieved through a trial-and-error process using the combination of the OpenFOAM® meshing utilities blockMesh and snappyHexMesh, as described by Segui et al. (2022).

To ensure sufficient data for comparison with experimental results, 26 cases were created for CFD simulation. For stirrer 1, velocities ranging from 550 to 1250 RPM were considered, while for stirrer 2, rates ranging from 400 to 950 RPM were examined, and for stirrer 3, velocities from 130 to 325 RPM were investigated. The torque and power number were obtained using the moment extracted from each blade.

In OpenFOAM®, the "forces" function object was utilized to calculate the forces and moments acting on specified patches. This calculation involves integrating pressure and viscous forces and moments, with the option to include resistance forces and moments from porous zones (OpenCFD Ltd, 2021). The data obtained from OpenFOAM® is stored in a ".dat" file containing six vectors per time step. The first three vectors represent pressure, viscous, and porous forces, while the last three represent pressure, viscous, and porous moments. To calculate the torque, the element of the shaft's axis from the fourth and fifth vectors (pressure and viscous moments) needs to be summed.

To analyze the data from the generated ".dat" files, a Python 3.10 algorithm was developed. This algorithm iterates through all 104 files, extracting the pressure and viscous moment vectors from the converged iterations' blade patches. Using Equation 4, the torque for each blade is calculated, and the total torque of the stirrer is determined by summing the torque values of all blades. The power consumption and power number are computed using Equations 5 and 6, respectively.

In Equation 4, $m\Gamma_{blade_n}$ represents the torque of the blade, m_{py} and $m_{\mu y}$ are the vector components of the moment pressure and viscous moment, P corresponds to power consumption, N denotes stirring velocity, P_0 signifies the power number, D represents the impeller diameter, and ρ indicates the density. The torque is obtained by summing the moments resulting from viscosity and pressure across the impeller surfaces, as explained by Fernandes Del Pozo et al. (2019). The resulting torque is multiplied by the density of the medium (approximately 1000 kg/m^3 for water) since the pressure values obtained from OpenFOAM® correspond to kinematic pressure for the case of incompressible solvers (static pressure divided by density).

$$m\Gamma_{blade_n} = m_{py} + m_{\mu y} \quad \text{(Eq. 4)}$$

$$P = 2\pi N m\Gamma \quad \text{(Eq. 5)}$$

$$P_0 = \frac{P}{D^5 * \rho * N^3} \quad \text{(Eq. 6)}$$

In addition to the CFD analysis mentioned earlier, **Journal Publication 6** proposes a novel concept for a two-stage covered lagoon anaerobic digester that utilizes wind energy for mixing. This concept addresses the scale issue of anaerobic digesters and offers a solution to Ireland's slurry disposal systems, which contributes to ozone layer depletion and methane emissions from animal manure.

The research approach outlined in **Journal Publication 6** includes conceptual design, analysis, and proposal of the new system. The proposition for retrofitting entails the transformation of open anaerobic lagoons into covered lagoons, offering a cost-effective alternative for farmers. The system offers several benefits by collecting the slurry from the barns and channelling it into a covered lagoon.

The conceptual design involves exploring the material for the tanks, the heating system, the mixing strategy, and what provides the mixing power. Table 3 shows the identification and planification of the conceptual design.

Table 3. Identification and planification.

Material	Heating	Mixing power	Mixing
Concrete	Boiler	Electric motor	Transversal
Soil	Small CHP	Wind-powered stirrer	Axial
Metal	Electric resistance	CHP	Pump
Membrane	Solar	Small CHP per stirrer	Kinetic energy from wind

From the matrix in Table 3, 256 possible system combinations are possible. Four of these 256 combinations are presented as the most viable options in Table 4. Option 1 involves a concrete floor for the covered lagoon, the heating system is powered by burning the biogas in a boiler or CHP unit, the mixing is performed with a pump, which is powered by a CHP unit fuelled with the biogas. For option 2 the floor is compacted soil based on the earth-lined slurry tanks guidance document (Scully et al., 2004) covered with an impermeable polyethylene membrane, the heating system is powered by burning the biogas in a boiler, the mixing power is obtained from the wind. Kinetic energy is harnessed from the wind and utilized to move the mixing system, composed of one or more axial stirrers. Option 3 utilizes only soil for the lagoon's floor. An electrical resistance provides heating, mixing with a pump, and a small CHP per pump. Option 4 is made out of metal, heated with an array of mirrors that utilize the sun, mixing power is obtained with solar energy, and the mixing strategy is with transversal stirrers.

Table 4. Optative configurations.

Configuration	Digester material	Heating system	Mixing power	Mixing
Option 1	Concrete	Burning the biogas	CHP	Pump
Option 2	Compacted soil covered with membrane	Burning the biogas	Kinetic energy from wind	Axial stirrer
Option 3	Soil	Electrical resistance	Small CHP per pump	Pump
Option 4	Metal	Solar mirrors array	Solar energy	Transversal

Figure 15 shows a schematic of the proposed stages of the system. Stages 1 and 2 are where the anaerobic digestion process occurs, and stage 3 is for storage.

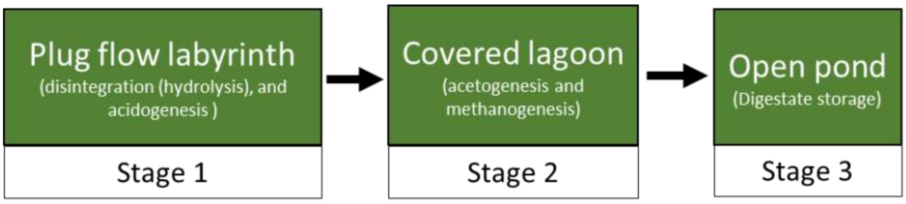


Figure 15. Proposed multistage anaerobic digester.

Firstly, the biogas generated from the slurry can be harnessed for producing electricity and/or heat, offering an alternative energy source. This reduces harmful emissions and creates potential revenue streams through the sale of excess biogas. Moreover, the produced heat can warm the covered lagoon, ensuring optimal anaerobic digestion conditions. Additionally, the electricity generated can power the barn or dairy plant, promoting energy efficiency.

Furthermore, the system allows for safely utilizing the digestate, the liquid-solid fraction remaining after digestion, as a nutrient-rich fertilizer for fields. This closed-loop approach minimizes waste and promotes sustainable agricultural practices. With its lower cost and scalability, the proposed system in **Journal Publication 6** offers a promising alternative for slurry disposal, addressing environmental concerns while providing economic benefits for farmers.

Figure 16 shows the manure flow in the system. The manure is collected from the barn, in case any other farm wastes are to be added to the anaerobic digester, these wastes need to be pasteurized. If not, it can be directly sent to a premixing and heating pre-treatment chamber, then passed to a plug flow labyrinth where the first two steps of anaerobic digestion (hydrolysis and acidogenesis) take place. Then it is passed to a covered lagoon where the acetogenesis and methanogenesis take place, and the biogas is produced. The next step is to dewater the digestate and send it to an open pond for storage until its spreading season.

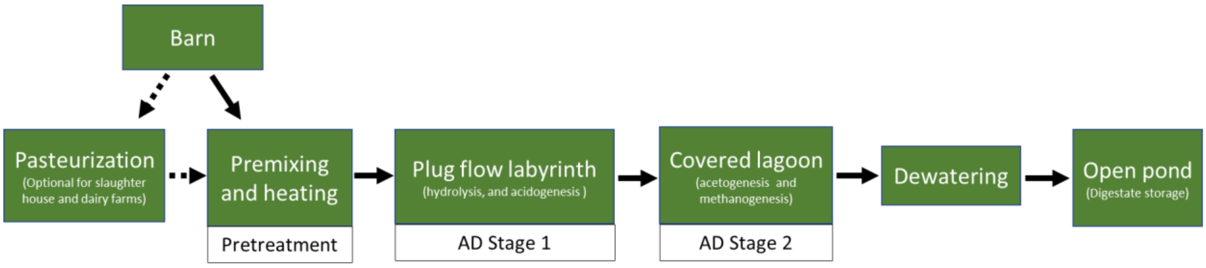


Figure 16. Manure flow in the system.

The research approach encompasses developing a comprehensive conceptual design for the two-stage covered lagoon anaerobic digester. This includes analyzing the system's requirements, such as the size and capacity needed to accommodate different farm sizes. The design also considers integrating wind energy for mixing within the covered lagoon, aiming to reduce operational costs and enhance system efficiency.

The system requirements include an efficient heating system with optimal temperature control, enabling the system to maintain ideal conditions for the anaerobic digestion process. Adequate mixing power is also essential to ensure proper digestion and homogeneity of the slurry. Furthermore, cost-effective materials that offer good durability and resistance to corrosive elements commonly found in the digestion process are necessary. Easy maintenance and operation are important aspects to consider, contributing to the system's reliability and longevity. Additionally, integrating renewable energy sources into the system is desirable to promote sustainability, reducing reliance on non-renewable energy and minimizing environmental impact.

Different attributes of the system were selected and evaluated to assess the various configurations of the anaerobic digestion system. Several criteria were considered to evaluate the options and determine the optimal choice for the system. These criteria include performance, economic viability, efficiency, reliability, scalability, ecological sustainability, and environmental risks.

To evaluate each configuration, a rating scale from 0 to 10 was used based on the following criteria:

- Performance: This criterion assesses how well each configuration meets the heating and mixing requirements of the anaerobic digester system, reflecting its effectiveness and efficiency in achieving optimal performance.
- Economic Viability: The overall economic feasibility of each configuration is considered, including cost-effectiveness, return on investment, and potential revenue generation.
- Efficiency: This criterion evaluates the energy efficiency of the heating and mixing mechanisms, measuring how effectively the system utilizes energy resources to minimize losses and maximize conversion.
- Reliability: The reliability and maintenance requirements of each configuration are considered, assessing the system's robustness, durability, and the frequency and complexity of maintenance tasks needed for uninterrupted operation.

- Scalability: The potential for the system to be scaled up or down to accommodate different farm sizes is considered, with a rating reflecting the ease and feasibility of adjusting the system's capacity to match varying slurry volumes.
- Ecological Sustainability: This criterion evaluates the environmental sustainability of each configuration, considering its impact on ecosystems, biodiversity, natural resources, and alignment with sustainable practices.
- Environmental Risks: The potential risks and negative impacts on the environment associated with each configuration are considered, with a rating reflecting the potential harm, pollution, or irreversible damage that could occur if the system is not managed correctly.

A comprehensive evaluation is conducted by assigning ratings from 0 to 10 to each criterion for every configuration. The option that receives the highest overall rating is considered the best choice, as it demonstrates superior performance, economic viability, efficiency, reliability, scalability, ecological sustainability, and low environmental risks compared to the other options. Figure 48 presents this evaluation in the form of a spider graph.

To obtain a representative size of the anaerobic digesters needed, data from six average Irish farms was taken from the “heavy soils programme” of Ireland’s Agriculture and Food Development Authority (TEAGASC, 2017). The data in Table 5 encompasses the herd size, air, and ground temperature. The daily biogas potential is calculated by multiplying the herd size by the daily manure per cow, times the biomethane potential of every kilogram of manure. Other methods for calculating are volatile solid content, chemical oxygen demand, methane yield potential, or biogas production model.

Table 5. Farm herd by size with an average air and soil temperature in degrees centigrade. Data extracted from TEAGASC (2017). Adopted from **Journal Publication 6**.

Farm	Herd Size (2019)	Temperature (°C)			
		Min (Feb)		Max (July)	
		Air	Soil	Air	Soil
Crossmolina	65	3.1	4.6	16.1	16.4
Lisselton	89	4.4	5.2	16.4	15.5
Kishkeam	100	2.6	3.6	16.2	15.4
Swan Cross	110	2.7	3.7	16.2	16.5
Ballinagree	120	2.9	4.5	16	16.6
Athea	130	3.4	4.6	15.7	15.4

The research also evaluates the retrofitting process of existing opened anaerobic lagoons to covered lagoons. This requires analyzing the structural modifications needed to ensure proper containment and optimize anaerobic digestion conditions. The economic feasibility and potential benefits of retrofitting are also investigated, considering cost savings and environmental impact.

Two larger farms with existing manure handling systems, with the possibility to be retrofitted, were visited. Both farms have open storage tanks (earth-lined slurry or tower tanks).

Farm 1 has a capacity for 1,100 cows. One Earth Lined Slurry (ELS) y tank of 15 x 40 x 4 m (2,036 m^3 volume) and a slurry tower of 42 m diameter x 3 m height (4,156 m^3 volume), holding up more than 6,000 m^3. This farm has a biogas potential of 560,000 m^3/year or 1,580 m^3/d. Premixing is possible with a pump in place. Figure 17 shows the existing infrastructure in farm 1, starting with the barn with scrappers, a slatted floor to collect the manure at a part of the barn, a mixing tank with a pump, an ELS tank, and a slurry tower tank.

Figure 17. Existing infrastructure in farm 1.

Farm 2 has a capacity for 600 cows. On the other hand, farm 2 has a capacity of 1,250 m^3 on the ELS tank and 640 m^3 on a second concrete storage tank. This farm has a biogas potential of 291,000 m^3/year or 798 m^3/d. The “barn” in this farm contains an underground tank beneath the slatted-floor cattle building.

Figure 18 shows farm 2, in the center, a satellite picture from the farm. Marked with green is the ELS tank, and marked with orange is the second storage tank. The stable marked with blue has a slurry collection system based on a slatted floor with underground storage.

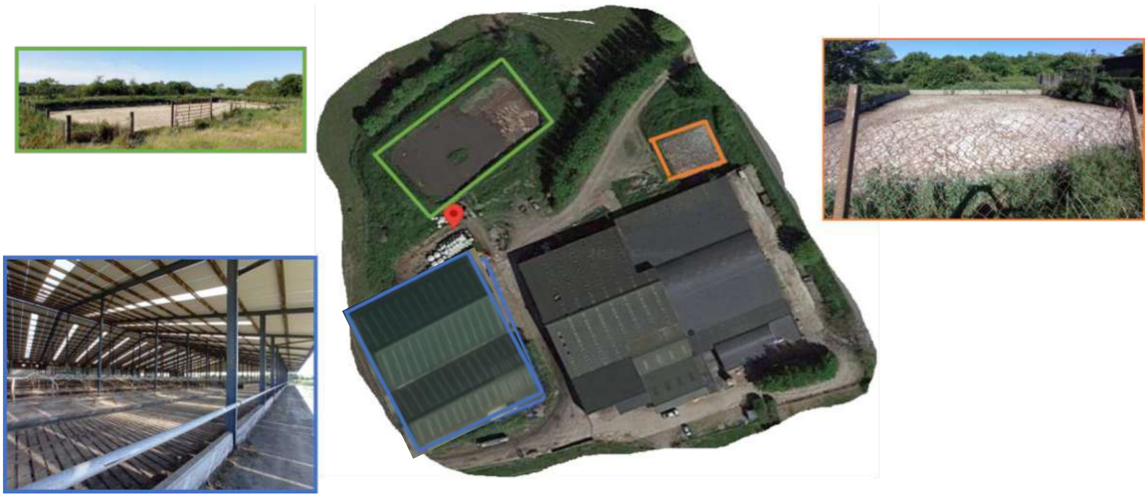


Figure 18. Existing infrastructure in farm 2.

Overall, the research approach presented in **Journal Publication 6** combines conceptual design, analysis, and proposal of a two-stage covered lagoon anaerobic digester system. By addressing the scale issue and providing a cost-effective alternative for slurry disposal, this innovative system offers potential solutions to environmental challenges faced by Irish farmers.

In addition to the extensive research conducted on various aspects of sustainable agricultural practices, including the development of a circular economy model for desert coastal regions, CO_2 utilization for greenhouse crop farming, CFD analysis in ALRs and CSTRs, and the retrofitting of slurry tanks to covered lagoons, the integration of a safe-by-design framework becomes a critical component to ensure the overall sustainability and safety of these systems. While these research pursuits have individually addressed specific challenges and proposed innovative solutions, incorporating safety considerations into the design process, as emphasized in **Journal Publication 7**, establishes a proactive and holistic approach towards creating secure and environmentally friendly agricultural and biorefinery operations. By integrating the principles of safe by design into the conceptualization, analysis, and implementation of these sustainable practices, the research collectively seeks to optimize resource utilization, minimize environmental impact, and protect the well-being of workers, thereby paving the way for a more sustainable and resilient future.

The research approach for **Journal Publication 7** focuses on developing a framework for safe by design in biorefineries. The objective is to shift the conventional approach, which tends to prioritize safety considerations at a later stage, by integrating safety considerations into the initial conceptual design phase. This approach aims to proactively identify and address potential safety issues, ensuring secure and sustainable biorefinery operations.

The research involves collaboration among various disciplines, including biotechnology, nanomaterials, and chemical engineering. These disciplines work together to implement comprehensive safety measures, considering specific concerns such as the containment of microorganisms and the prevention of cross-contamination in feedstocks. By employing rigorous protocols, the research aims to mitigate risks and ensure the safe operation of biorefineries.

A comprehensive framework of Safe by Design for biorefineries should include the following components:

1. Hazard Identification: thoroughly assess potential hazards associated with biorefinery processes, including chemicals, materials, and activities that may pose risks to workers, the environment, and the surrounding community.
2. Risk and Reliability Assessment: evaluate the likelihood, severity, and reliability of identified hazards and potential failures within the biorefinery system. Consider factors such as exposure pathways, toxicity, consequences of failures, and the overall reliability of equipment and processes.
3. Design Integration: incorporate safety considerations into the early stages of biorefinery design, ensuring that safety features and measures are integrated into the overall process design. Consider aspects like process layout, equipment selection, and material compatibility while prioritizing risk reduction and reliability enhancement.
4. Inherent Safety: implement inherently safer design principles to minimize or eliminate hazards at the source rather than relying solely on protective measures. Design processes and equipment that inherently reduce the potential for accidents, such as using less hazardous materials or eliminating the need for hazardous processes.
5. Control Measures: develop and implement engineering controls, administrative controls, and personal protective measures to mitigate identified risks. This may include ventilation systems, containment systems, safety interlocks, standard operating procedures, training programs, and personal protective equipment.
6. Monitoring, Maintenance, and Reliability Management: establish a comprehensive monitoring and maintenance program to continuously assess the biorefinery system's performance, reliability, and safety. Regular inspections, preventive maintenance, reliability-centered maintenance, and equipment reliability assessments are essential to ensure ongoing safety and minimize the risk of failures.
7. Emergency Preparedness: develop emergency response plans and procedures to handle potential incidents or accidents effectively. This includes establishing communication protocols, training personnel on emergency response, conducting drills, and ensuring the availability of appropriate emergency equipment and resources.
8. Compliance and Auditing: regularly evaluate and audit the biorefinery's safety practices to ensure compliance with relevant regulations, standards, and best practices. Identify areas for improvement and ensure continuous adherence to safety protocols through internal audits and external assessments.
9. Communication and Training: ensure effective communication of safety policies, procedures, and expectations to all stakeholders, including workers, contractors, and neighboring

communities. Regular training programs should be conducted to enhance safety awareness, promote a culture of safety, and provide specific training on handling hazardous materials and operating equipment safely.

10. Continuous Improvement and Total Quality Management: foster a culture of continuous improvement by implementing principles from total quality management and lean manufacturing methodologies. Encourage employee involvement in identifying safety improvement opportunities, implementing corrective actions, and promoting a proactive safety and reliability enhancement approach.

By incorporating these elements, a comprehensive framework of Safe by Design for biorefineries can help identify and mitigate potential hazards, ensure the safety of workers and surrounding communities, enhance system reliability, and promote the sustainable and responsible operation of biorefinery processes.

The research approach compiles different safe-by-design strategies into a safe-by-design biorefinery framework. These strategies include probabilistic risk-based design, deterministic (safety factor-based) design, fail-safe design, active safe design, passive safe design, vandal-proof design, idiot-proof (or fool-proof) design, fault-tolerant design, and circular design. Through a comprehensive analysis of these strategies, the research aims to determine the most effective approaches for integrating safety considerations into the conceptual design process of biorefineries.

Overall, the research approach for **Journal Publication 7** encompasses the development of a comprehensive framework for safe by design in biorefineries. Through interdisciplinary collaboration, evaluating different safe-by-design strategies the research aims to prioritize safety considerations from the early stages of conceptual design, thereby establishing secure and sustainable biorefinery operations.

In summary, this thesis adopts a comprehensive research approach that combines various methodologies and techniques, including theoretical analysis, CFD simulations, case studies, data analysis, conceptual modeling, and proposal of new concepts. The aim is to explore and evaluate multiple aspects of the circular bioeconomy within chemical engineering. By examining resource utilization, waste management, and sustainable practices, this research seeks to provide valuable insights and practical solutions that contribute to a more sustainable and environmentally friendly future. Moving forward to the results section, the findings from these rigorous investigations will be presented, revealing the outcomes of the applied methodologies and their implications for advancing the circular bioeconomy in chemical engineering.

Chapter 5. Results and Discussion

In the previous section, the research approach and background of the publications relevant to the objectives of this thesis have been identified. This section contains the results from the publications divided into seven sections. Section 1 presents the results of the circular economy model, section 2 the optimal greenhouse areas for CO_2 crop enrichment, section 3 the hydrodynamics of air lift reactors, section 4 the power consumption of continuously stirred tank reactors, section 5 retrofitting existing infrastructure for the bioeconomy and section 6 the safety considerations when designing and operating a biorefinery. Finally, this chapter ends with a summary.

5.1. Circular economy model

For developing the circular economy model proposed in **Journal Publication 1,** different technologies from the Atacama and Sonoran Deserts and non-existing well-known bioeconomy applications were integrated. Solar energy is utilized to power a desalination plant, the freshwater is then used for food production either with hydroponic systems or water dozing with hydrogels provided by an irrigation system. Seaweed can be produced in the sea to be utilized either for food or to produce biochemicals. Seawater is also used for microalgae production in air lift photobioreactors or raceway ponds. The waste streams are separated depending on their salinity and then processed through anaerobic digestion, where biogas and digestate are produced. The biogas can then be upgraded to biomethane, and the carbon dioxide fraction is utilized as a feed for the microalgae, or it can be burned in a CHP unit; the exhaust gas, composed mainly of carbon dioxide, can also be utilized as feed for the microalgae, and the energy can be utilized as energy supply for the desalination plant. The digestate can then be used as fertilizer for the food production systems, and nutrients, such as nitrogen, phosphates, and potassium, can be recovered from the digestate. Figure 19 shows the circular economy model just described above.

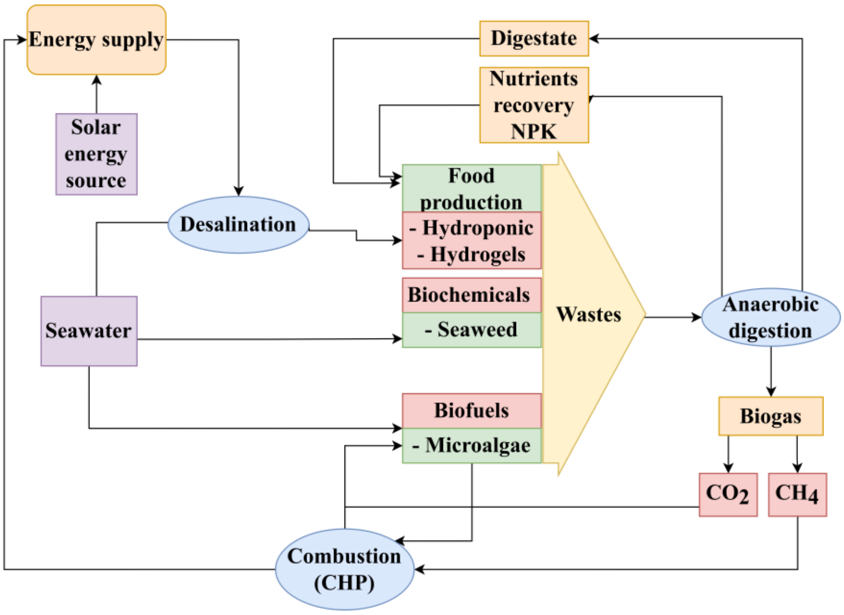


Figure 19. Circular economy model. Adopted from **Journal Publication 1**.

As described in the research approach, the attributes associated with the processes and products were assessed by evaluating them from 0 to 10, where zero indicates poor performance, and ten indicates outstanding performance. The four attributes considered in the evaluation were technology readiness level, economic viability, ecological sustainability, and environmental risks. The technology readiness level assessed the readiness of the technology for deployment, while ecological sustainability evaluated its environmental impacts. Environmental risks refer to the potential irreversible environmental damage if the products or processes are not managed correctly, and economic viability evaluates the capital costs. The spider graph in Figure 20 evaluates the technologies in the circular economy model described above.

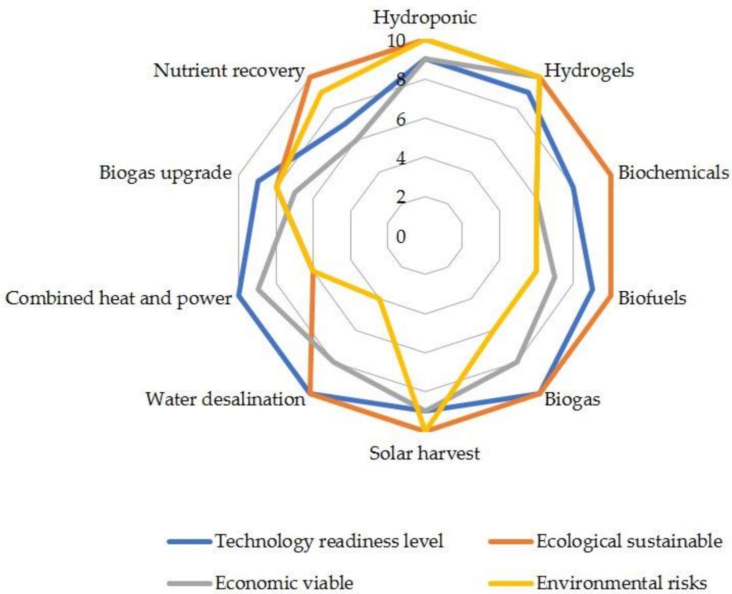


Figure 20. Attribute evaluation of technologies utilized in the circular economy model. Adopted from **Journal Publication 1**.

The new perspective proposed with this circular economy model is presented in Figure 21, where the standard opinion and reality in desert coastal regions concerning water scarcity are used to develop a new hypothesis on utilizing the circular economy principles applied to the synergetic integration of state-of-the-art technologies. The state-of-the-art technologies are in most cases already in place in these regions. From here a new perspective promoting mature technologies such as, water desalination, solar energy, anaerobic digestion, hydroponic farming, water dosing with hydrogels applied on irrigation systems, microalgae and seaweed farming and nutrient recovery from anaerobic digestion is presented.

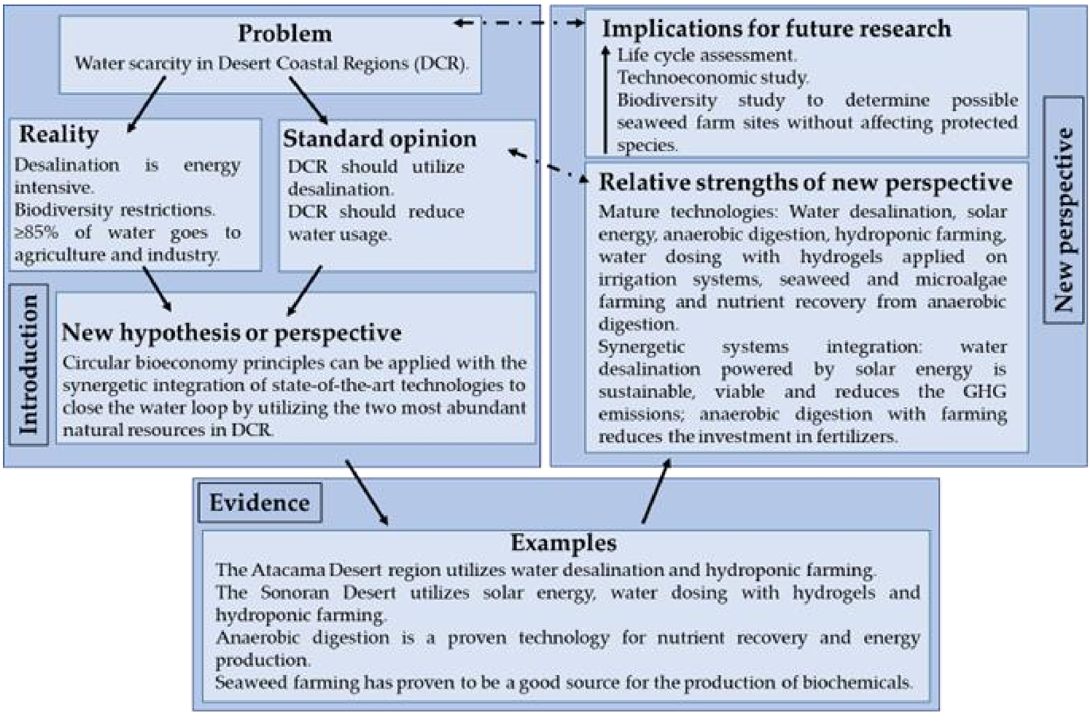


Figure 21. Process followed to develop the new perspective. Adopted from **Journal Publication 1.**

5.2. CO_2 enrichment for greenhouse crop farming

In **Journal Publication 2**, a biomethane plant located in Lower Austria was utilized to propose food production in greenhouses with CO_2 enrichment. The Bruck an der Leitha biomethane plant generates annually 5,200,000 m^3 of biogas from waste. From which 3,300,000 m^3 are upgraded to biomethane and 1,900,000 m^3 is unutilized carbon dioxide. Biomethane is obtained by upgrading biogas through a purification process. The different biogas upgrading technologies and their distribution through European biogas plants is presented in Chapter 3 of **Public Report 2,** appended to this thesis. This plant utilizes a membrane upgrading technology that Makaruk et al. (2010) developed. Since there is no use for the carbon dioxide in this plant, it is released into the atmosphere. Based on the circular economy principles, resources should not be wasted; hence the reutilization of this wasted resource (CO_2) is proposed for the enrichment of greenhouses.

The methodology employed in this study includes analyzing data, performing calculations, and comparing greenhouse areas across various designs. Two different methods were utilized for optimal greenhouse size calculation, a simplified and a detailed calculation.

As described in the schematic representation (Figure 4) of the simplified calculation in the research approach, the monthly availability of sun hours determines the number of available hours for utilizing CO_2 in greenhouse crop production. Table 6 shows the monthly CO_2 enrichment obtained by multiplying the CO_2 applied rates (Blom et al., 2002) for a completely closed and a partially opened greenhouse. These monthly values are added and divided by the yearly available CO_2 to obtain the greenhouse area in hectares that can be enriched with carbo dioxide.

Table 6: Potential yearly CO_2 use by month based on sunshine hours at Bruck an der Leitha. Adopted from **Journal Publication 2**.

Month	Number of hours applied (h)	CO_2 Applied Rate (kg/ha/h)					
		Completely Closed			Partially Opened		
		12	18	24	45	65	90
January	275.9	3,310.8	4,966.2	6,621.6	12,415.5	17,933.5	24,831
February	288.4	3,460.8	5,191.2	6,921.6	12,978	18,746	25,956
March	372	4,464	6,696	8,928	16,740	24,180	33,480
April	411	4,932	7,398	9,864	18,495	26,715	36,990
May	471.2	5,654.4	8,481.6	11,308.8	21,204	30,628	42,408
June	480	5,760	8,640	11,520	21,600	31,200	43,200
July	483.6	5,803.2	8,704.8	11,606.4	21,762	31,434	43,524
August	440.2	5,282.4	7,923.6	10,564.8	19,809	28,613	39,618
September	375	4,500	6,750	9,000	16,875	24,375	33,750
October	334.8	4,017.6	6,026.4	8,035.2	15,066	21,762	30,132
November	276	3,312	4,968	6,624	12,420	17,940	24,840
December	260.4	3,124.8	4,687.2	6,249.6	11,718	16,926	23,436
Total (kg)		53,622	80,451	107,244	201,082.5	290,452.5	402,165
Greenhouse Area (Ha)		17.92	11.95	8.96	4.78	3.31	2.39

The process for the detailed calculation is presented in Figure 5 of the research approach. Table 7 shows the hectares that can be enriched with CO_2 with and without CO_2 storage for a completely closed greenhouse and for double polyethylene and standard glass partially opened greenhouse.

Table 7: Summary of results. Adopted from **Journal Publication 2**.

Concept	Completely Closed	Partially Opened: Double Polyethylene	Partially Opened: Standard Glass
Greenhouse with No CO_2 Storage (Ha)	7.03	4.82	2.81
Greenhouse with CO_2 Storage (Ha)	11.31	6.97	3.85
CO_2 Storage (m^3)	368,989	276,515	232,791
CO_2 Uptake Rate ($kg/h/100m^2$)	0.12-0.24	0.25-0.35	0.5-0.6

5.3. Hydrodynamic study in air lift bioreactors with computational fluid dynamics

The first step when performing CFD is evaluating the spatial discretization error. This validation process involves conducting mesh convergence studies, as discussed and shown in the research approach section.

Not all of the CFD studies in ALRs are presented in this section; a timeline of all the works is shown in Figure 22. From Figure 22, the CFD studies performed chronologically in ALRs are the following. First, **Public Report 2**, followed by a poster for a summer school based on the results of **Public Report 2.** The subsequent two studies showed three different vessels' morphology with single and double draft tube configurations presented in **Journal Publication 3** and **Poster 3**. This was followed by an open-source toolbox in **Public Report 3**, where a tutorial based on **Journal Publication 3** was presented. The following study was **Journal Publication 4**, where different draft tube configurations were tested for double-stage ALRs. The last study in the timeline is **Conference Publication 1**, where single, double, and triple-stage configurations were compared.

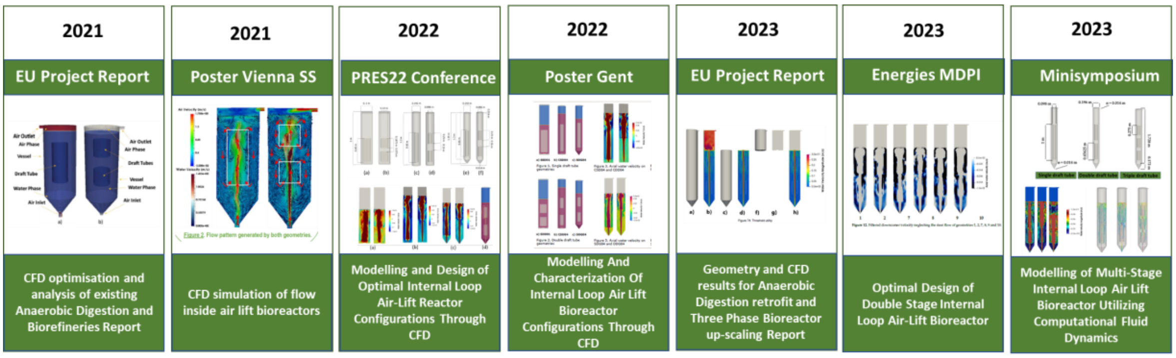


Figure 22. Timeline of works in air lift reactors during the thesis. Adapted from Ramonet et al. (2023).

The first part of the study in air lift reactors for this thesis is **Journal Publication 3**. The mesh properties utilized in this publication are presented in Table 8, which are the number of cells, maximum skewness, and maximum non-orthogonality.

Table 8: Mesh properties.

Properties	Squared Single Draft Tube	Squared Double Draft Tube	Cylindrical Single Draft Tube	Cylindrical Double Draft Tube	Single Draft Tube Geometry	Double Draft Tube Geometry
Cells	672,172	681,806	320,430	641,705	445,808	645,772
Maximum Skewness	4.21	4.41	3.2	4.48	4.71	3.26
Maximum Non-orthogonality	53.96	52.50	63.56	64.80	55.29	53.51

The results from the simulations are presented in Table 9. The first column notes if it is the squared, cylindrical, and cylindrical connect bottom geometries, the second column marks if it is a single or double draft tube configuration, and the third column indicates if the velocity is 0.01, 0.02, or 0.04 m/s. The simulation time for all geometries was 60 seconds. In **Journal Publication 3**, the same table shows the cases from the squared double draft tube at 0.02 m/s and cylindrical single draft tube at 0.04 m/s, both at less than 35 seconds of simulation time, since computation was not completed at the time of the submission. The computation time varied from 59 to 3,123 hours. The number of cores utilized for the computation was either 4 or 8; for more details, consult **Journal Publication 3**. The timestep chosen for the simulation is shown in the last column; in some cases, it was set as an adjustable timestep, which means that it is self-calculated by the algorithm depending on the Courant number.

Table 9: Summary from computation. Adapted from **Journal Publication 3**.

Geometry	Draft tube	Velocity ($x10^{-2}$ m/s)	Computation Time (h)	Timestep (s)
Squared	Single	1	650	$5x10^{-4}$
	Single	2	797	$5x10^{-4}$
	Double	1	656	$5x10^{-4}$
	Double	2	3,123	$1x10^{-4}$ *
Cylindrical	Single	4	2,898	$1x10^{-4}$ *
	Double	1	198	$1x10^{-3}$
	Double	4	207	$1x10^{-3}$
Cylindrical coned bottom	Single	4	59	$1x10^{-3}$ *
	Double	4	81	$1x10^{-4}$ *

* Adjustable timestep, self-calculated by the algorithm depending on the timestep's Courant number.

Figure 23 shows the six geometries in (a) squared single and double draft tube, (b) cylindrical single and double draft tube, and (c) cylindrical coned bottom single and double draft tube at 60, 26.1 and 60 seconds of simulation, respectively. Figure 23 (d) shows the two draft tube circulation loops; yellow is the circulation loop for the first draft tube, and green is the circulation loop for the second draft tube for the double draft tube configuration.

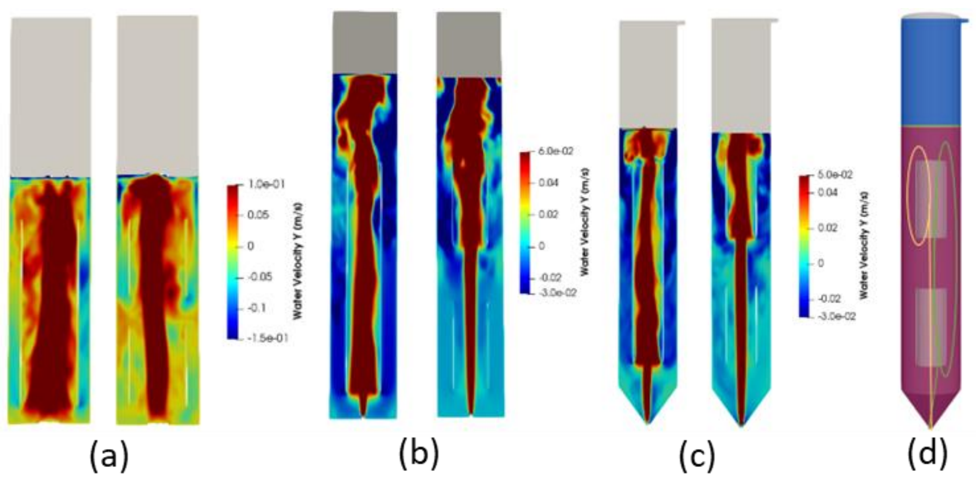


Figure 23. Squared (a), cylindrical (b), and cylindrical conned bottom (c) geometries, (d) circulation loops. Adopted from **Journal Publication 3**.

Table 10 presents the results from the nine cases simulated in **Journal Publication 3**. In Table 10, two sampling points were taken on the downcomer side of the reactor: one at the bottom, between the bottom and the draft tube, and another at the top, between the draft tube and the fluid's level. The table displays the sampled points' turbulence kinetic energy, fluid velocity, and pressure. Despite using lower velocities for the inlet in geometries Squared Single Draft Tube and Squared Double Draft Tube, higher downcomer velocities are observed at the bottom sampled point due to the pressure increase caused by the reactor diameter-to-draft tube diameter ratio. The Cylindrical Single Draft Tube and Cylindrical Double Draft Tube geometries exhibit lower turbulent kinetic energy at both the top and bottom points, which can be attributed to the distance between the top of the draft tube and the liquid's surface area. Regarding the draft tube loop circulation time, the worst performance is observed in Cylindrical Double Draft Tube with an inlet velocity of 0.04 m/s.

Table 10: Obtained results. Adopted from Ramonet et al. (2022a).

Case			**Turbulence kinetic energy in fluid phase (m^2/s^2)**		**Fluid velocity on Y-axis (m/s)**		**Pressure (mbar)**		**Draft tube loop circulation time (s)**	
Geometry	**Draft tube**	**Velocity** ($x10^{-2}$ m/s)	Top	Bottom	Top	Bottom	Top	Bottom	First	Second
Squared	Single	1	5.87×10^{-4}	1.36×10^{-4}	0.028	0.02	1,127	1,182	16.56	-
	Single	2	2.02×10^{-4}	8.24×10^{-5}	0.04	0.07	1,269	1,321	12.28	-
	Double	1	6.73×10^{-4}	2.82×10^{-5}	0.018	0.02	1,125	1,180	34.85	54.22
	Double	2	3.22×10^{-4}	2.29×10^{-6}	0.04	0.006	1,045	1,097	24.76	32.37
Cylindrical	Single	4	6.18×10^{-5}	1.95×10^{-6}	0.035	0.019	1,004	1,074	145.36	-
	Double	1	1.44×10^{-4}	1.36×10^{-6}	0.007	0.001	1,004	1,095	27.52	45.04
	Double	4	2.21×10^{-4}	7.52×10^{-7}	0.043	0.001	1,004	1,077	20.70	146.06
Cylindrical coned bottom	Single	4	4.48×10^{-5}	2.14×10^{-6}	0.018	0.006	1,004	1,077	53.40	-
	Double	4	1.28×10^{-4}	1.04×10^{-6}	0.033	0.007	1,004	1,077	26.91	110.76

Figure 24 plots the squared geometry's riser and downcomer water velocity with single and double draft tube configurations at 0.01 and 0.02 m/s. On the lower part of the single and double draft tube cases at 0.02 m/s, the riser behaves very similarly, but at around 1/3 of the vessel, it can be seen that the double draft tube configuration reaches a higher water velocity. On the upper part of the reactors there is a big difference in the upcomer (riser) water velocities. On the other hand, on the downcomer velocities, there is a big difference between the single and the double draft tube configurations on the lower part of the reactor, which is not seen on the top section of the reactor. A one order of magnitude difference can be seen between the riser and downcomer water velocities.

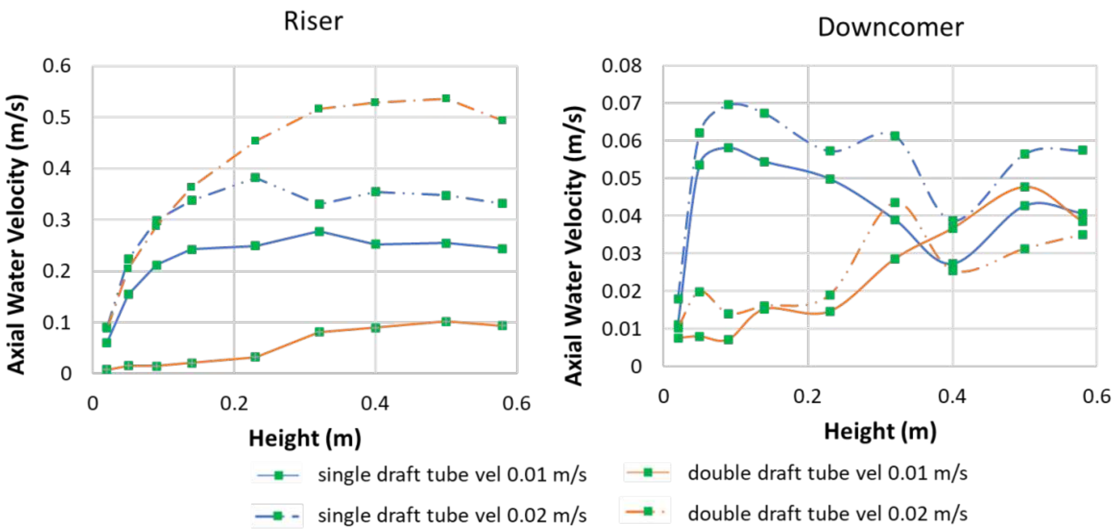


Figure 24. Riser and downcomer velocity of squared geometry. Adopted from Ramonet et al. (2022a).

Figure 25 plots the riser and downcomer velocities of the cylindrical geometry with single and double draft tube configurations. The single draft tube configuration was simulated at 0.04 m/s inlet velocity, while the double draft tube configuration was simulated at 0.01 and 0.04 m/s inlet velocity. The behavior of the single and double draft tube configurations is quite similar on the riser at 0.04 m/s. The double draft tube configuration at 0.01 m/s does not show the same trend as the others on the riser section, and the velocity on the top of the reactor is higher when utilizing this inlet velocity. When analyzing the downcomer velocities, the double draft tube configurations show the same behavior at the lower part of the reactor, but a big difference can be seen in the upper section. The single draft tube configuration shows a stable downcomer velocity due to the fact that the flow behaves as a pipe flow in most of the reactor; a significant pressure drop (more than 50 %) can be seen when the draft tube finishes in the lower part of the reactor.

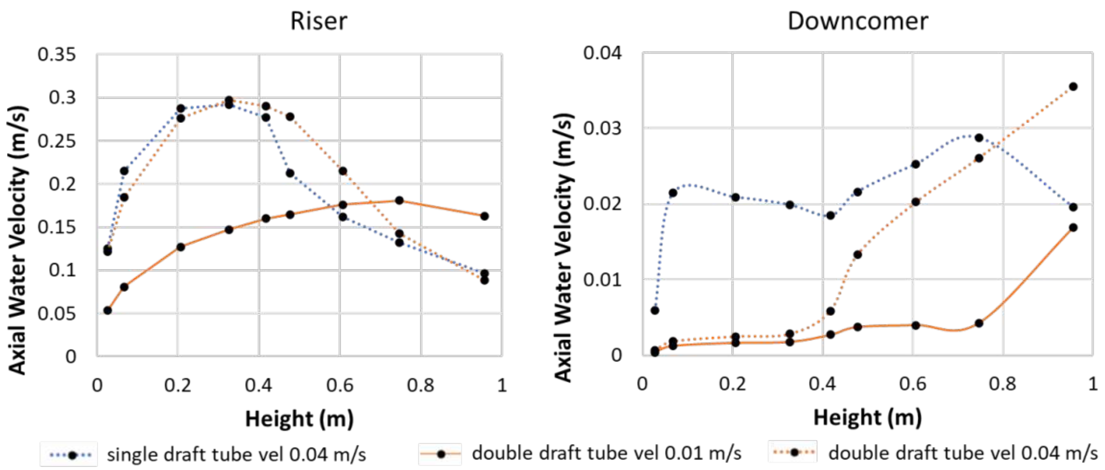


Figure 25. Riser and downcomer velocity of cylindric geometry. Adopted from Ramonet et al. (2022a).

Figure 26 plots the cylindrical conned bottom geometry with single and double draft tube configurations at 0.04 m/s. Both geometries show the same behavior from the riser section, but higher velocities are seen on the double draft tube configuration. On the downcomer velocities, higher velocities are seen on the top of the reactor on the double draft tube, but then drops at 3/4 of height, and the single daft tube configuration remains more stable with a higher velocity.

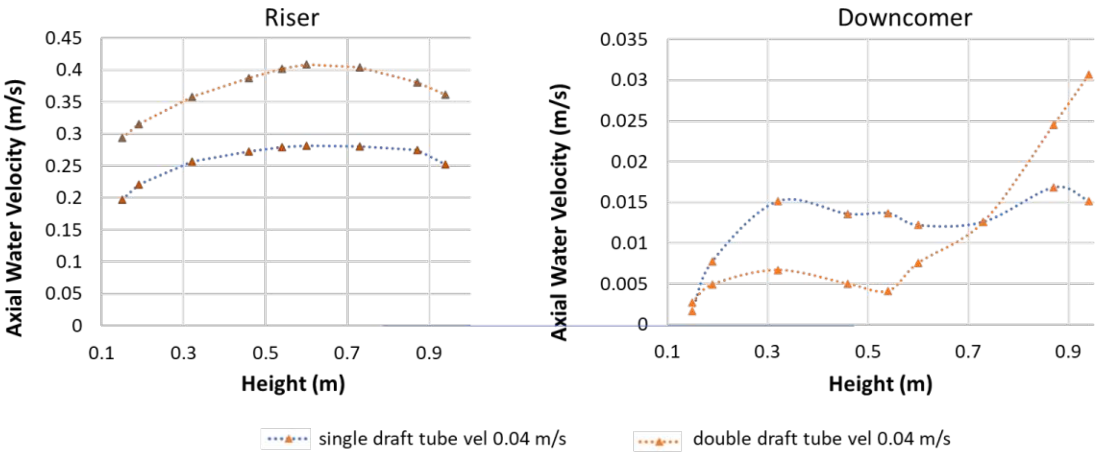


Figure 26. Riser and downcomer velocity of cylindrical coned bottom geometry. Adopted from Ramonet et al. (2022a).

Figure 27 plots the riser velocity of the squared, cylindrical, and cylindrical conned bottom with single and double draft tube configurations at all simulated velocities. The axis with the axial water velocity was set the same on the three graphs for comparison reasons. This figure shows that the higher upcomer (riser) velocity is higher on the squared geometries, followed by the cylindrical conned bottom geometries. The higher velocities on the squared geometries can be by the pressure difference created by the vessel-draft tube ratio and the distance between the interphase surface and the end of the draft tube area, as reported in **Journal Publication 3**.

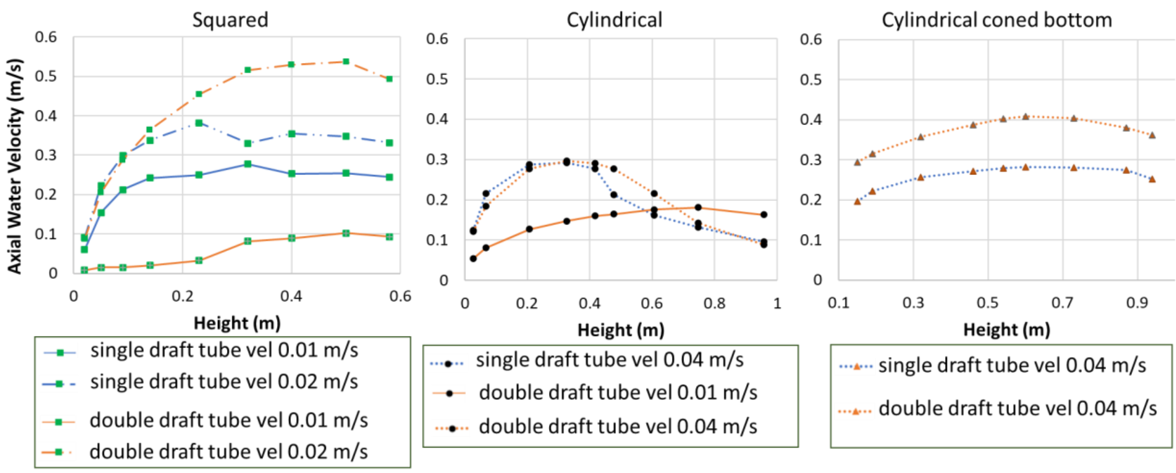


Figure 27. Axial water velocities on the riser of squared, cylindrical, and cylindrical coned bottom geometries. Adopted from Ramonet et al. (2022a).

Figure 28 plots the downcomer velocity of the squared, cylindrical, and cylindrical conned bottom with single and double draft tube configurations at all simulated velocities. The axis with the axial water velocity was set the same on the three graphs for comparison reasons. When comparing all the simulated cases from this study, the higher downcomer velocities at the bottom part of the air lift reactors is seen on the squared single draft tube cases. The tendency presented on the cylindrical and cylindrical coned bottom double draft tube geometries downcomer velocities shows a smoother trend at the bottom of the reactor.

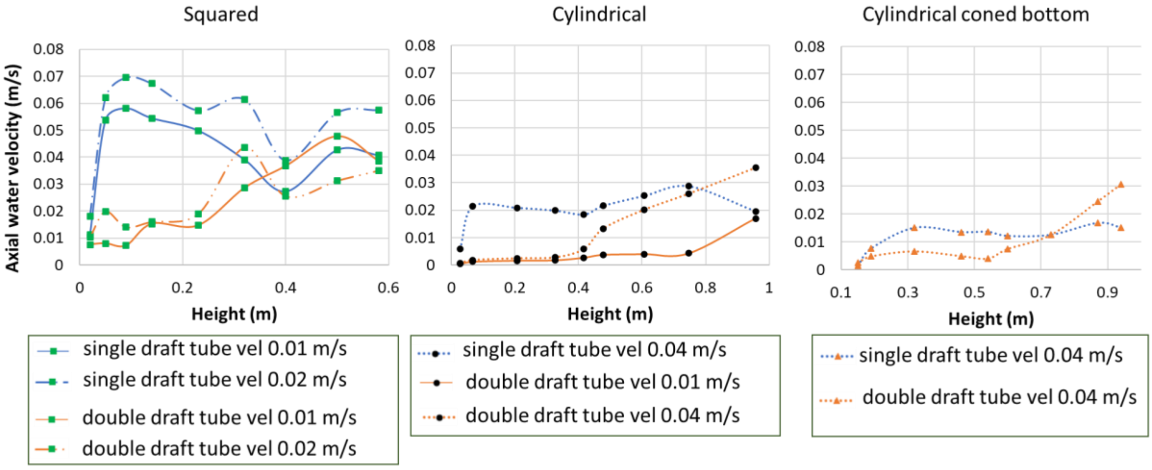


Figure 28. Axial water velocities on the downcomer of squared, cylindrical, and cylindrical coned bottom geometries. Adopted from Ramonet et al. (2022a).

As highlighted in **Journal Publication 3**, it is essential to allocate more attention to understanding the impact of dividing the draft tube into two or more sections on the overall mixing inside ALRs. This study aimed to compare various internal configurations of ALRs using CFD. The square single and double draft tube reactors exhibited higher downcomer velocities, greater turbulence kinetic energy, and shorter loop circulation times among the three geometries examined. When comparing single and double-draft tube configurations, it was observed that the upper part of the double-draft tube design experienced higher turbulent kinetic energy. The ratio of draft tube-vessel width and the distance between the draft tube and the fluid's surface was found to impact the loop circulation time of the draft tube. Additionally, the internal geometry of ALRs was found to influence the downcomer velocity. Further research is necessary to investigate the flow behavior when different draft tube parameters are utilized, such as distance between draft tube and surface, distance between draft tubes, length of draft tubes, and draft tube diameter.

The second part of the study in air lift reactors for this thesis is **Journal Publication 4**. As described in the research approach, ten geometries were utilized for this study based on the cylindrical and cylindrical coned bottom from **Journal Publication 3**.

Figure 29 shows the ten geometries utilized in this study. Geometries 1 and 3 are the same as the cylindrical double draft tube and cylindrical conned bottom double draft tube geometries presented in **Journal Publication 3**. Figure 29 was already shown on the research approach as Figure 9, but it is brought up again to illustrate the ten geometries. Specifics from the geometries can be consulted on the appended **Journal Publication 4**. Geometry two was made as a variation of geometry one by varying the distance between draft tubes, geometry four was created as a variation of three by also varying the distance between draft tubes, and geometries five and six are geometries three and four but with different liquid height to investigate how this parameter affects the overall flow inside the ALR. Geometry seven has the same draft tube heights as one; the difference is that the upper part of both draft tubes has a reduction in diameter, giving the draft tubes the appearance and properties of funnels. Geometry nine has the same particularity as seven, but the draft tubes are placed at the same height as geometry two. Geometries eight and ten are also variations of geometry two; on eight, the top draft tube is inverted from the one in nine. Geometry ten keeps the top draft tube as geometry two, but the bottom one has a funnel configuration as in eight and nine.

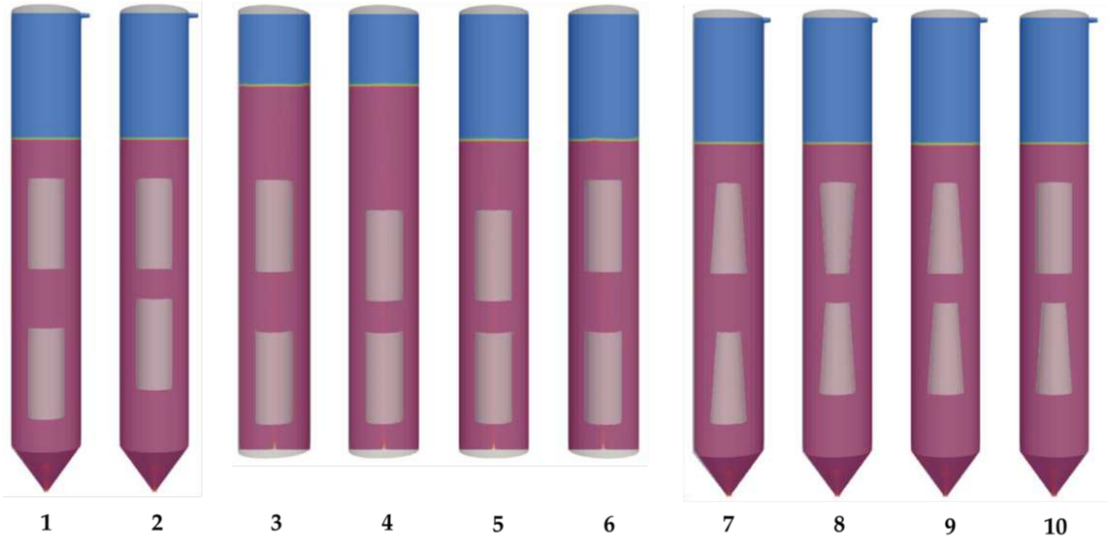


Figure 29. Ten geometries utilized in the study. Extracted from **Journal Publication 4**.

The mesh properties utilized in this publication are presented in Table 11, which are the number of cells, maximum skewness, and maximum non-orthogonality. The skewness is defined as “the difference between the shape of the cell and the shape of the equilateral cell of equivalent volume” (Zhou et al., 2022).

Table 11. Mesh properties of double-stage ALR geometries utilized for **Journal Publication 4**. Adopted from **Journal Publication 4**.

Geometry	Cell Number (×10^3)	Max. Skewness	Max. Non-Orthogonality
1	646	3.27	53.51
2	646	2.51	64.66
3	642	4.48	64.80
4	306	3.74	64.86
5	306	3.74	64.86
6	642	4.48	64.80
7	623	2.80	64.83
8	1,012	2.84	54.85
9	683	3.15	46.39
10	1,043	3.37	58.38

The first comparison of the geometries can be performed with geometries one and two. Figure 30 plots the riser and downcomer of geometries one and two. This figure shows that varying the distance between cylindrical draft tubes does not have significant effects on the overall flow of ALRs.

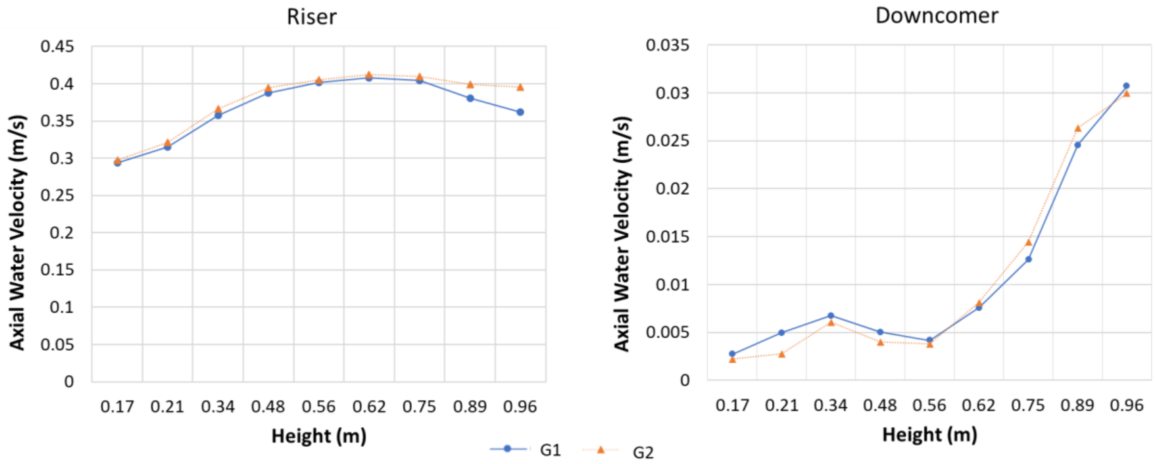


Figure 30. Riser and downcomer velocity for geometries 1 and 2. Adapted from **Journal Publication 4**.

The second comparison is made with the cylindrical geometries three, four, five, and six. Figure 31 plots the riser and downcomer velocities of the cylindrical geometries based on the cylindrical double draft tube geometry from **Journal Publication 3**, taken initially from Shi et al. (2021). As it can be seen from Figure 31, the axial velocity shows the same trend on the riser section on all four geometries. Geometries 5 and 6 exhibit higher rising velocities at the bottom of the draft tube, while the axial velocity on the riser section remains approximately the same across all four cases. Upon leaving this section, geometries 5 and 6 show higher velocities again. Geometries 3 and 4, with the same liquid height, exhibit a similar trend. Regarding geometrical characteristics, geometry 3 and 6 share the same features, differing only in liquid height, while geometry 4 and 5 have the same geometrical characteristics but different liquid heights. Figure 31 demonstrates that the behavior of the riser is mainly influenced by the fluid height, as geometries with the same liquid height exhibit similar tendencies. Moving on to the downcomer velocities shown in Figure 31, they exhibit a consistent pattern at the bottom of the reactor but vary in the upper part. Geometry 3 shows a linear decrease in velocity as the flow descends, while geometry 5 demonstrates a more stable velocity in the upper part, which could be advantageous for microorganism cultures. Considering that the variations in these four cases involve liquid height and the distance between draft tubes, the most stable downcomer velocity is observed when the bottom clearance and distance between the draft tubes are approximately equal, and their sum is roughly equal to the top clearance.

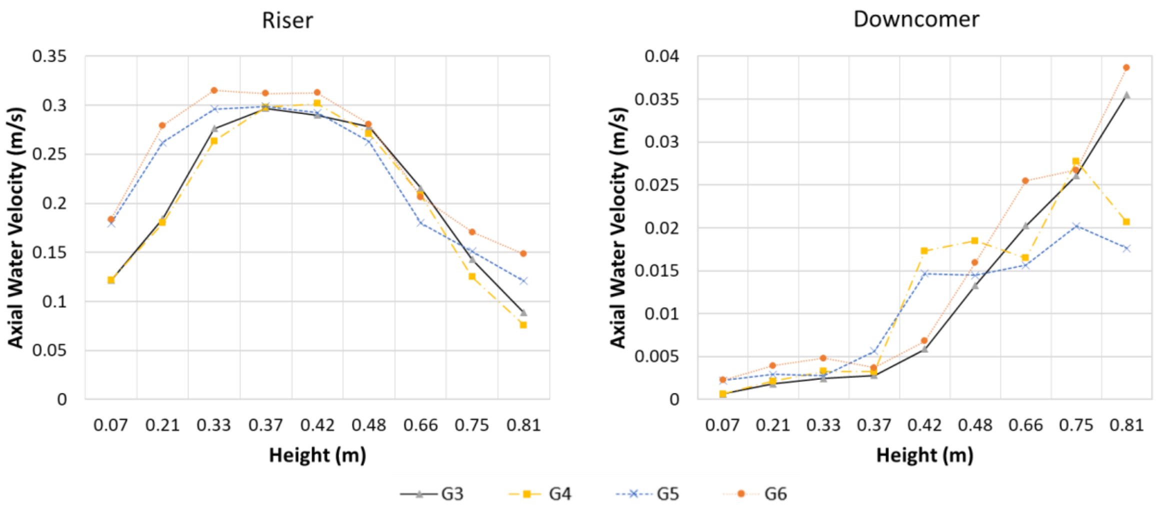


Figure 31. Riser and downcomer velocity for geometries 3, 4, 5, and 6. Adapted from **Journal Publication 4**.

Figure 32 plots the riser and downcomer velocities of the cylindrical coned bottom geometries based on the cylindrical coned bottom double draft tube geometry from **Journal Publication 3**. Figure 32 shows that geometry 7 exhibits poorer performance compared to the other three cases in the upper half of the reactor, as it has a lower riser velocity. Geometries 8 and 10 display similar behavior in the riser, although geometry 8 demonstrates a higher velocity at the top of the reactor, which may be attributed to the contraction-expansion effect. In terms of the downcomer velocities, all geometries exhibit a similar trend at the bottom of the reactor. However, at the top of the reactor, geometry 9 the velocity is approximately the double of geometries 8 and 10 and nearly triples the velocity of geometry 7. Geometry 7 demonstrates greater stability in the liquid phase of the top half of the reactor for downcomer velocity, but it exhibits the lowest velocity in the same region for the riser.

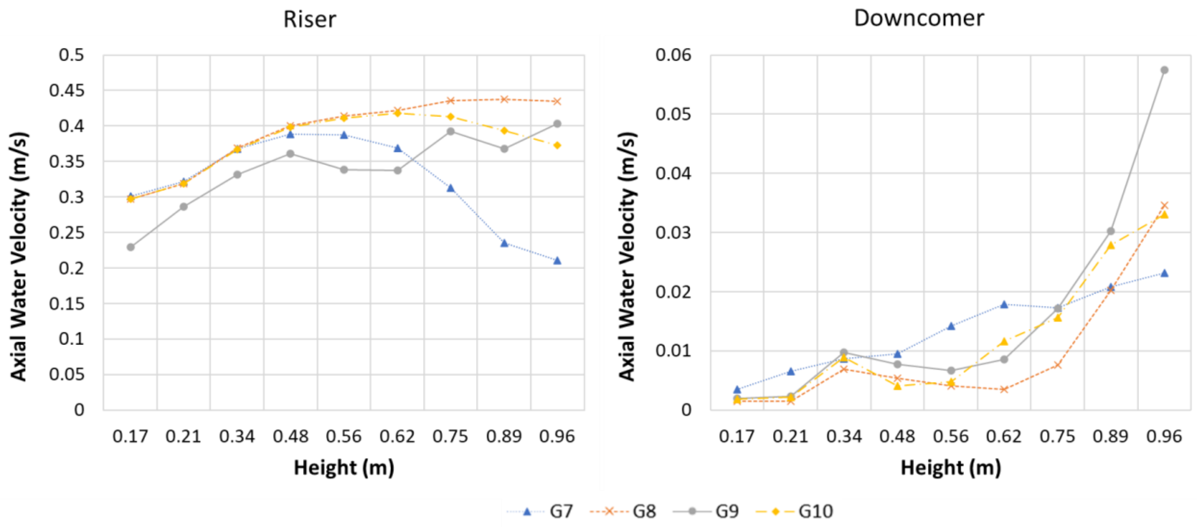


Figure 32. Riser and downcomer velocity for geometries 7, 8, 9, and 10. Adapted from **Journal Publication 4**.

The results from the simulations are presented in Table 12. Two data extraction points were chosen at approximately the same height on each case's top and bottom of the downcomer side. The pressure varies across cases depending on the liquid height. The axial velocity is shown as an absolute value in meters per second (m/s). Table 12 also provides information on turbulent kinetic energy. The circulation time of the draft tube was calculated for each case. All simulations were performed on four cores, with computation times ranging from 81 to 438 hours, and an adjustable time step was utilized in all cases.

Table 12 includes two columns labeled "first draft tube" and "second draft tube." The "first draft tube" column indicates the time it takes for a particle to travel from the inlet, move up until the top draft tube is reached, descend, and incorporate itself back into the flow of the first draft tube, forming a loop as shown in Figure 10 with the blue arrows. The "second draft tube" column indicates the time it takes for a particle to travel from the inlet, ascend to the interphase section, and descend to the bottom of the lower draft tube, forming a loop, as shown in Figure 10 with the black arrows.

Moving from geometry 1 to 2 involved raising the draft tube by 8 cm, a change also made in geometries 7 to 9. Previous literature, such as the work by Pironti et al. (1995), has experimentally studied this phenomenon using a single draft tube geometry with a conical bottom, revealing that draft tube placement significantly affects the hydrodynamic behavior. Analyzing the data in Table **12**, it can be observed that the top velocity in geometry 9 is more than twice that of its reference geometry (7), which can be attributed to the double velocity gradient achieved by the smaller distance between the draft tubes and the double funnel configuration. On the other hand, the downcomer velocity is one-third of its counterpart, resulting in a less active zone at the bottom of the reactor. Among the six configurations with conical bottoms, geometry 9 exhibits the fastest recirculation loop in the upper loop of the reactor (top draft tube). The fastest circulation for the second loop in the conical bottom geometries was observed in geometry 7. As for the cylindrical draft tube (geometries 1 and 2), the only notable remark is the decrease in velocity at the bottom of the reactor at the measuring point caused by the movement of the draft tube.

The conical bottom reactor demonstrates the following characteristics when compared by reactor type. Cases 1, 2, 7, 8, 9, and 10 exhibit similar pressure and draft tube loop circulation times, with pressure ranging from 100,374 to 100,402 Pa and draft tube loop circulation time on the first loop ranging from 21.4 to 36.97 s. However, there are noticeable differences in axial velocity and turbulent kinetic energy. Cases 1 and 2 have the highest values for turbulent kinetic energy, while cases 9 and 10 have the highest values for axial velocity. Case 8 has the highest value for turbulent kinetic energy and the second-highest value for axial velocity. Case 7 has the lowest values for axial velocity and turbulent kinetic energy. Overall, it appears that the design parameters used in cases 1, 2, 8, 9, and 10 were more effective in achieving high axial velocities and turbulent kinetic energies than the design parameters used in case 7.

Among the four cylindrical ALR cases (3, 4, 5, and 6). Cases 3 and 6 have the same geometry but different liquid heights. Similarly, cases 4 and 5 have the same geometry but different liquid heights. Specifically, the liquid heights in cases 3 and 4 are identical, while those in cases 5 and 6 are the same. However, the liquid heights in cases 3 and 4 differ from those in cases 5 and 6. Looking at the results, case 3 demonstrates the highest axial velocity (at the bottom), turbulent kinetic energy (at the bottom), and second lowest circulation time for the first draft tube loop. Case 4 exhibits the second lowest axial velocity and turbulent kinetic energy (at the top). Case 5 has the second highest turbulent kinetic energy for the top section. Case 6 has the lowest circulation time for the second draft tube loop, indicating the most efficient flow in this loop. In summary, case 6 displays the most efficient fluid circulation and mixing, followed by case 3, case 5, and finally, case 4.

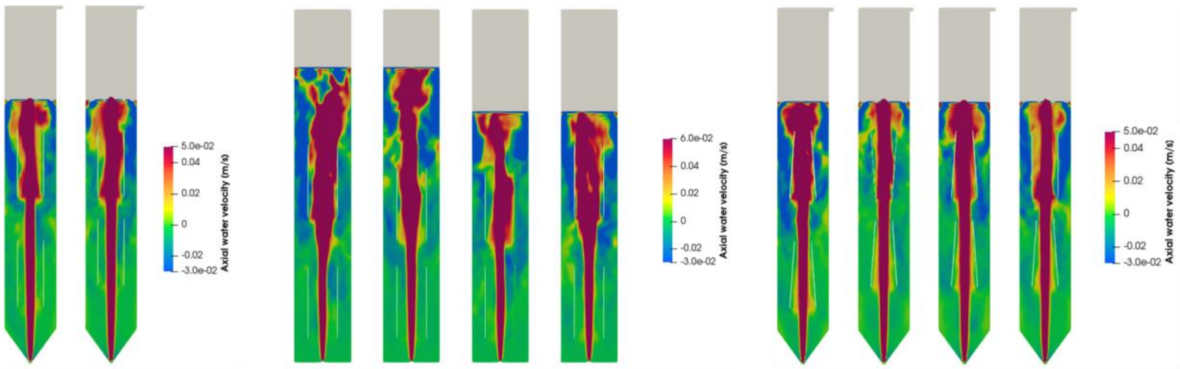
Table 12. Results from the simulations.

Geometry	**Pressure (Pa)**		**Axial Velocity (m/s)**		**Turbulent Kinetic Energy (m^2/s^2)**		**Draft Tube Loop Circulation Time (s)**	
	Top	**Bottom**	**Top**	**Bottom**	**Top**	**Bottom**	**First**	**Second**
1	100,388	107,722	0.0307	0.0049	1.24×10^{-4}	1.04×10^{-6}	27.02	110.76
2	100,389	107,721	0.0299	0.0027	1.27×10^{-4}	7.99×10^{-7}	25.07	128.04
3	100,395	107,727	0.0355	0.0024	2.21×10^{-4}	7.36×10^{-7}	20.7	146.06
4	100,401	107,732	0.0206	0.0032	7.26×10^{-5}	9.96×10^{-7}	21.4	112.17
5	100402	106,268	0.0176	0.0029	1.20×10^{-4}	1.04×10^{-6}	23.81	104.77
6	100,396	106,266	0.0386	0.0039	1.57×10^{-4}	1.82×10^{-6}	18.59	91.75
7	100,388	107,723	0.0232	0.0062	5.95×10^{-5}	9.20×10^{-7}	24.45	73.48
8	100,387	107,721	0.0346	0.0015	3.04×10^{-4}	8.27×10^{-7}	36.97	156.27
9	100,374	107,707	0.0574	0.0023	5.90×10^{-4}	1.05×10^{-6}	21.63	98.41
10	100,388	107,721	0.0331	0.0022	6.11×10^{-5}	8.66×10^{-7}	23.58	110.58

Figure 33 illustrates the axial velocity distribution for all ten cases. The comparison is divided into three sections, similar to the previous section: the first comparison includes geometries 1 and 2

(Figure 33a), the second comparison includes geometries 3-6 (Figure 33b), and the third comparison includes geometries 7-10 (Figure 33c). In the visualization, positive values from orange to red represent the riser velocity, while negative values from green to blue represent the downcomer velocity.

In geometries 1 and 2 (Figure 33a), it can be observed that the downcomer flows into the bottom of the draft tube. This counterflow pattern is also present in most geometries shown in Figure 33b. However, this counterflow effect has been eliminated by modifying the bottom draft tube into a funnel shape, reducing the diameter of the upper part of the draft tube, as depicted in Figure 33c.



a) b) c)

Figure 33. Axial water velocities of double-stage internal loop ALRs simulated. A) geometries 1 and 2, b) geometries 3, 4, 5, and 6, and c) geometries 7, 8, 9, and 10. Adopted from **Journal Publication 4**.

As an illustrative example, to represent the flow, geometry 9 is presented every 5 seconds from 5 to 60 seconds, coloring the axial water velocity in m/s with a maximum of 0.05 m/s in the upcomer and a maximum of 0.03 in the downcomer. Figure 34 shows this representation.

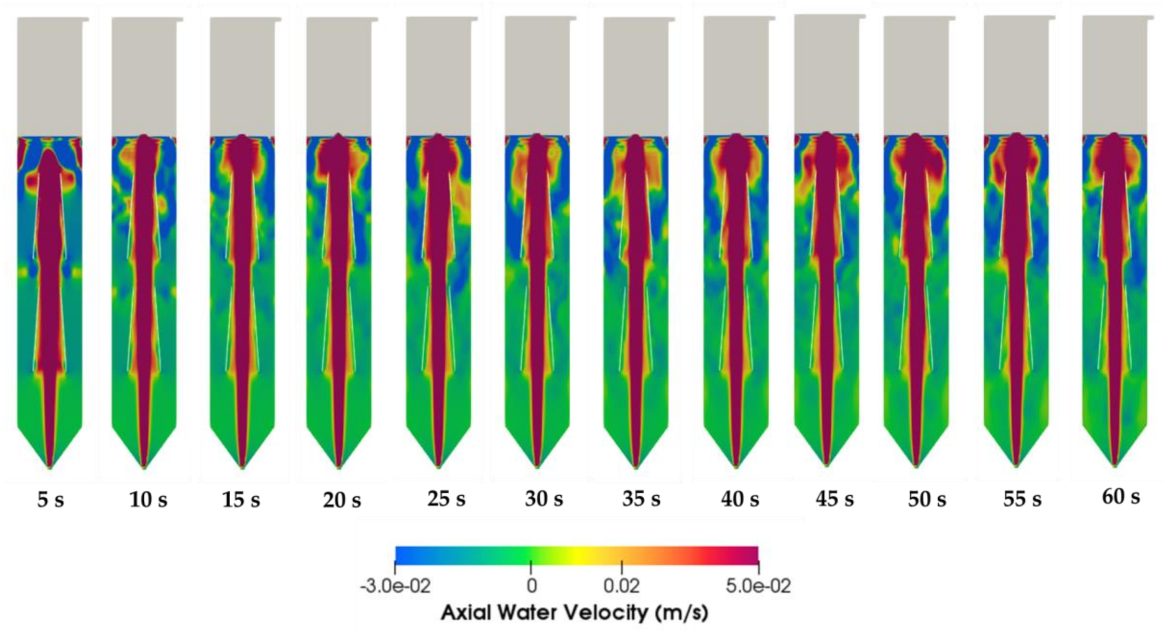


Figure 34. Axial water velocity of Geometry 9. Adopted from **Journal Publication 4**.

To obtain a visual representation of the downcomer velocity, all coned bottom geometries (1, 2, 7, 8, 9, and 10) are presented in Figure 35, coloring the values from 0 to -0.01 m/s (blue to black) by neglecting the positive axial water velocity, only the downcomer velocity is colored.

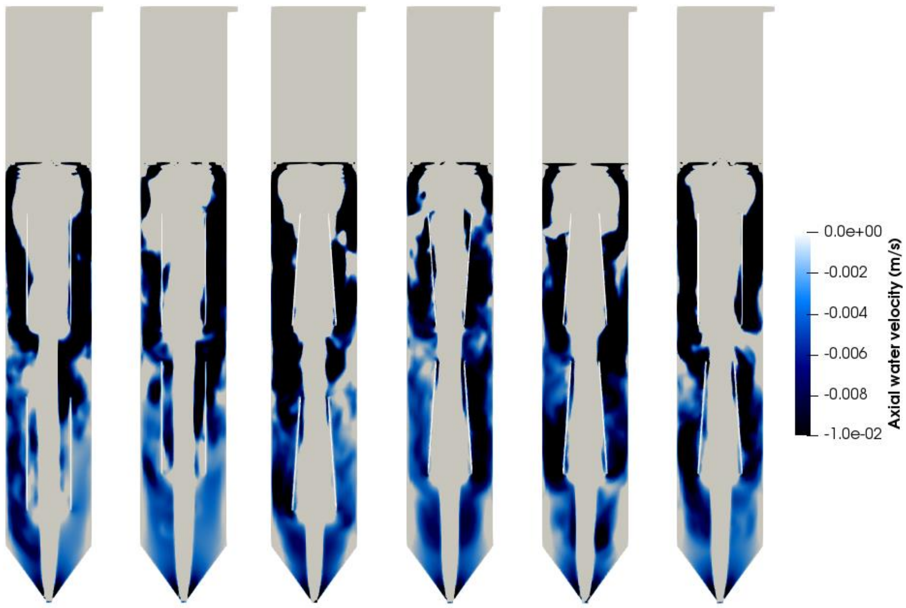


Figure 35. Downcomer velocity of geometries 1, 2, 7, 8, 9 and 10. Adopted from **Journal Publication 4**.

Figure 36 illustrates the flow patterns within air lift bioreactors, where 25 particles were selected as a sample to visualize streamlines colored according to their velocity magnitude. As shown from Figure 36, most of the particles stay in the first circulation loop and the 25 particles during the

60 seconds of simulation cannot capture the second loop in all cases. The velocity distribution shows higher velocities on the top of the reactor.

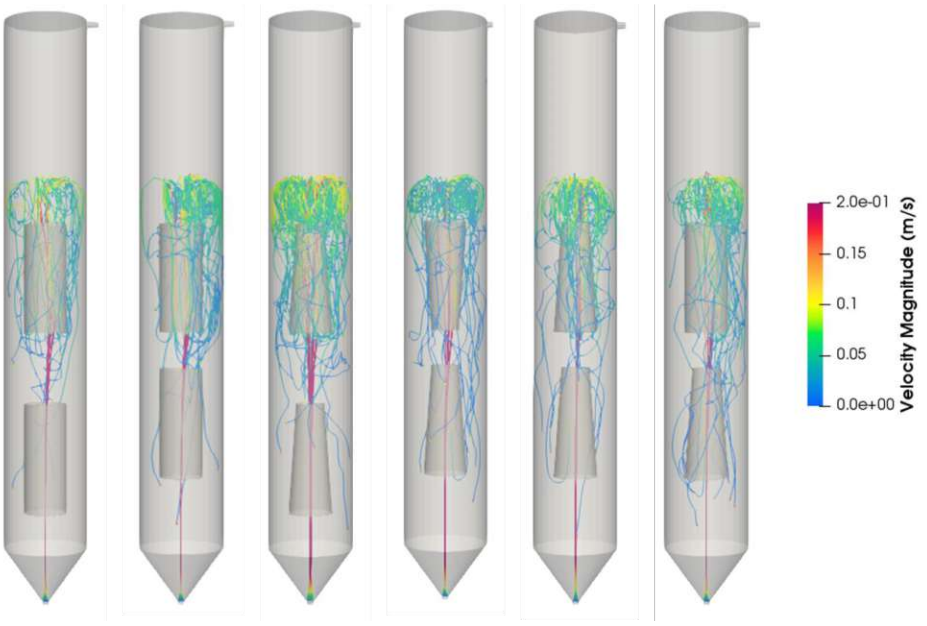


Figure 36. Streamlines coloring the velocity in m/s of geometries 1, 2, 7, 8, 9, and 10. Adopted from **Journal Publication 4**.

As a validation of the two-fluid model, the squared single draft tube geometry from Jia et al. (2007) was compared to the simulations performed in **Journal Publication 3**. Figure 37 shows this comparison.

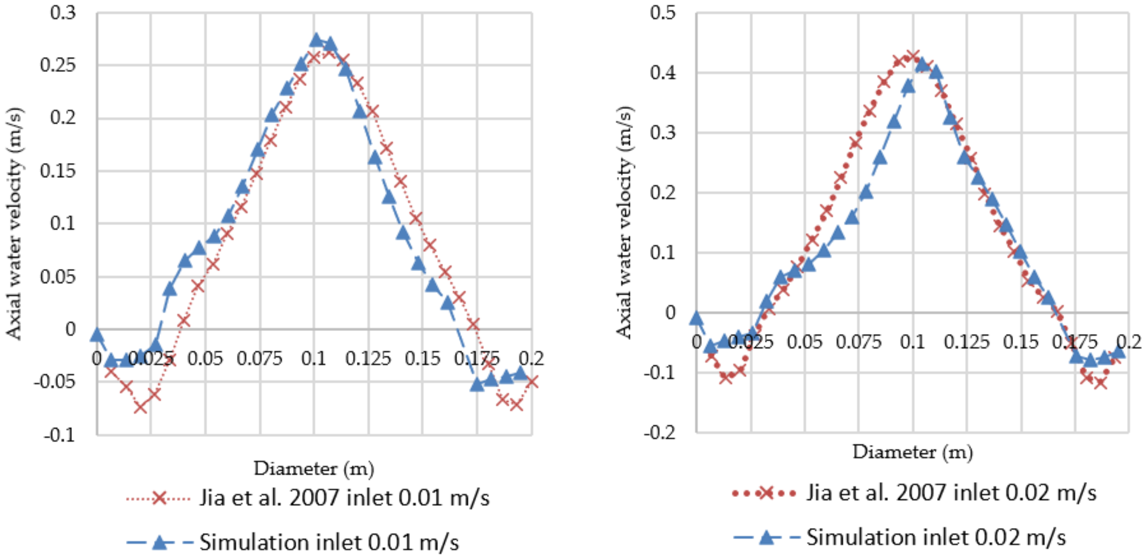


Figure 37. Model validation from literature values for 0.01 and 0.02 m/s. Adapted from **Journal Publication 4**.

Continuing with the hydrodynamics in internal loop air lift reactors, **Conference Publication 1** compares the hydrodynamics of the single (SDG), double (DDG), and triple (TDG) draft tube configurations. Figure 38 shows the velocities in the riser section of the reactor. Among the configurations, the single draft tube geometry exhibits the highest riser velocity, followed by the double and triple draft tubes.

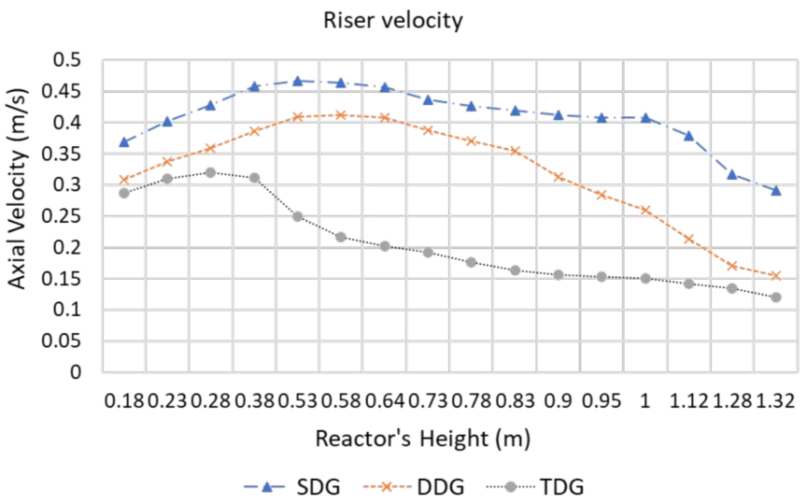


Figure 38. Comparison of riser velocity of Single Draft tube Geometry (SDG), Double Draft tube Geometry (DDG), and Triple Draft tube Geometry (TDG). Adapted from **Conference Publication 1**.

Figure 39 shows the downcomer velocities, revealing that the single draft tube configuration maintains a consistent downcomer velocity along the draft tube. The triple draft tube geometry demonstrates the least steep slope. When comparing the reactor height values for each configuration, it is observed that at the height of 0.18 meters, the TDG configuration has the highest value (4.55×10^{-3}) compared to SDG (1.96×10^{-3}) and DDG (1.93×10^{-3}). However, at a height of 0.28 meters, SDG exhibits the highest value (3.17×10^{-2}) compared to DDG (8.08×10^{-3}) and TDG (1.37×10^{-2}). At higher reactor heights (above 0.5 meters), the values for all three configurations become more comparable, with only slight differences between them.

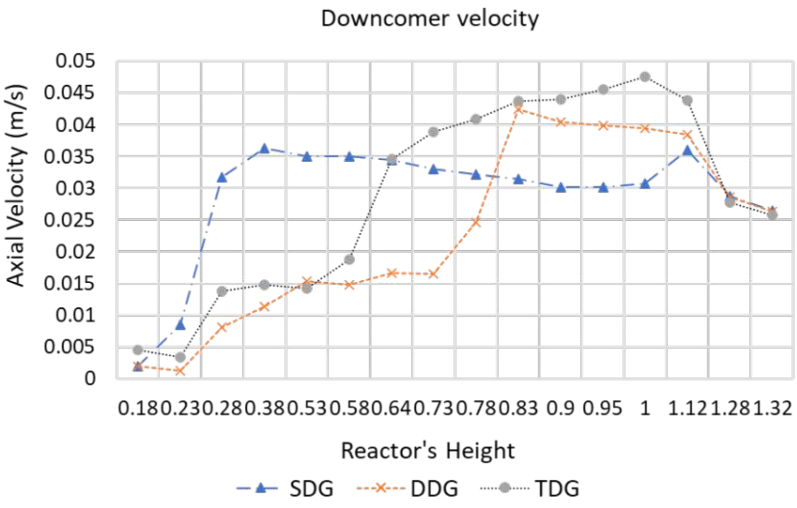


Figure 39. Comparison of riser and downcomer velocity of Single Draft tube Geometry (SDG), Double Draft tube Geometry (DDG), and Triple Draft tube Geometry (TDG). Adapted from **Conference Publication 1**.

Overall, the data suggest that the internal configuration of the air lift reactor significantly influences its performance, with each configuration demonstrating unique strengths and weaknesses at different reactor heights.

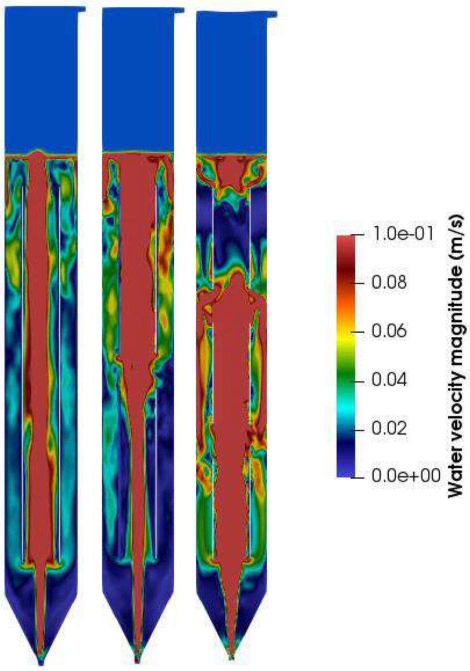
Table 13 presents simulation results for the three different geometries: single draft tube (SDG), double draft tube (DDG), and triple draft tube (TDG). The results include pressure values, turbulent kinetic energy in the fluid phase, and fluid velocity on the Y-axis. At a height of 0.23 meters, the pressure values are similar for all three geometries. As the height increases, the pressure values decrease slightly across all configurations. Regarding turbulent kinetic energy, at a height of 0.23 meters, SDG exhibits the highest value, while at an altitude of 0.58 meters, TDG has the highest value. At heights of 0.78 meters and 0.95 meters, DDG shows the highest turbulent kinetic energy, and at 1.32 meters, TDG has the highest value. In terms of fluid velocity on the Y-axis, TDG demonstrates the highest values at a height of 0.23 meters, while SDG has the highest velocity at a height of 0.58 meters. At heights of 0.78 meters and 0.95 meters, TDG maintains the highest fluid velocity, whereas, at 1.32 meters, all configurations have similar velocities. These findings emphasize the influence of draft tube geometry on pressure, turbulent kinetic energy, and fluid velocity, with variations observed at different heights within the system.

Overall, the data suggests that the different draft tube geometries impact the pressure, turbulent kinetic energy, and fluid velocity within the system. The values vary depending on the height of the reactor and the specific geometry being considered. These findings highlight the importance of considering the draft tube design when analyzing the performance and characteristics of the system, as each configuration exhibits its own strengths and weaknesses at different heights.

Table 13. Simulation results from **Conference Publication 1**. Adapted from Ramonet et al. (2023).

	Pressure (Pa)			Turbulent kinetic energy in fluid phase (x10^{-6} m^2/s^2)			Fluid velocity on Y-axis (x10^{-2} m/s)		
Height	**SDG**	**DDG**	**TDG**	**SDG**	**DDG**	**TDG**	**SDG**	**DDG**	**TDG**
0.23	111,044	111,048	111,098	3.949	0.999	1.468	0.858	0.121	0.342
0.58	107,623	107,626	107,676	2.792	5.019	9.666	3.497	1.475	1.874
0.78	105,668	105,671	105,721	4.382	16.568	11.175	3.217	2.463	4.086
0.95	104,006	104,009	104,058	7.774	9.551	71.622	3.015	3.987	4.552
1.32	100,386	100,389	100,440	108.579	109.766	113.069	2.647	2.638	2.580

To illustrate the fluid circulation loops, Figure 40a shows the water velocity magnitude of the three geometries. To focus only on the downcomer velocity, the riser velocity was also neglected by coloring the axial water velocity from 0 to -0.025 m/s, limiting the minor value for visualization purposes in Figure 40b. At limited downcomer velocities, it is observed that the double-stage geometry exhibits a higher downcomer velocity in the top section. At the same time, the triple-stage configuration shows a more stable downcomer velocity.



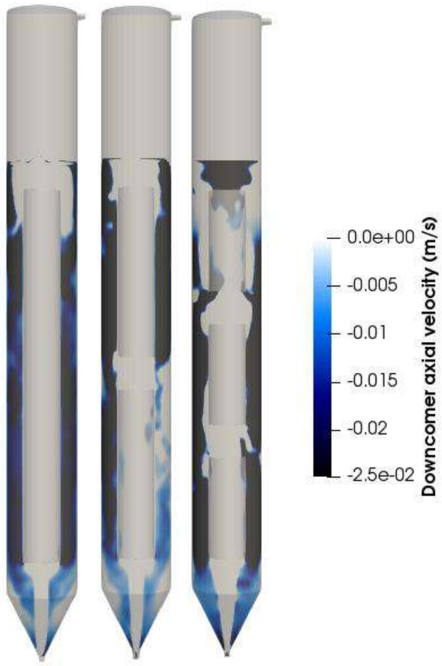


Figure 40. a) Water velocity magnitude of single, double, and triple draft tube geometries colored at a maximum velocity of 0.1 m/s. b) Downcomer velocity of single, double, and triple draft tube geometries colored at a maximal downcomer velocity of 0.025 m/s. Adopted from **Conference Publication 1**.

Part of this research was coupling an in-house Lagrangian particle utility to the two-fluid model (Euler-Euler approach). Figure 41 shows the particles at 7, 15, 33, and 75 seconds.

Figure 41 shows the distribution of injected particles at various time intervals across the three different geometries. The particles, injected through the inlet patch at a constant flow rate, have a total mass of 5 kg and are released for one second at a velocity of 0.06 m/s with 4994 parcels per second. Notably, the conical bottom in Figure 41 (a), (b), (c), and (d) is a region with minimal fluid circulation, resulting in particle stagnation, as it is typically utilized for sedimentation. Experimental observations in reactors with conical bottoms have shown the accumulation of solids, which could account for the observed disparity, as suspended solids may precipitate within the reactor (Garcia-Calderon et al., 1998). At 7 seconds of simulation (Figure 41a), it can be seen that the particles in the SDG have reached the surface, while not on the other two geometries; at this time, it can also be seen that the particles escape from the openings between the draft tubes. At 15 seconds of simulation (Figure 41b), all geometries have particles that have reached the surface. At 33 seconds (Figure 41c), all the geometries have particles that have reached the bottom of the reactor. Finally, at 75 seconds (Figure 41d) of simulation, the particles in all geometries seem more dispersed.

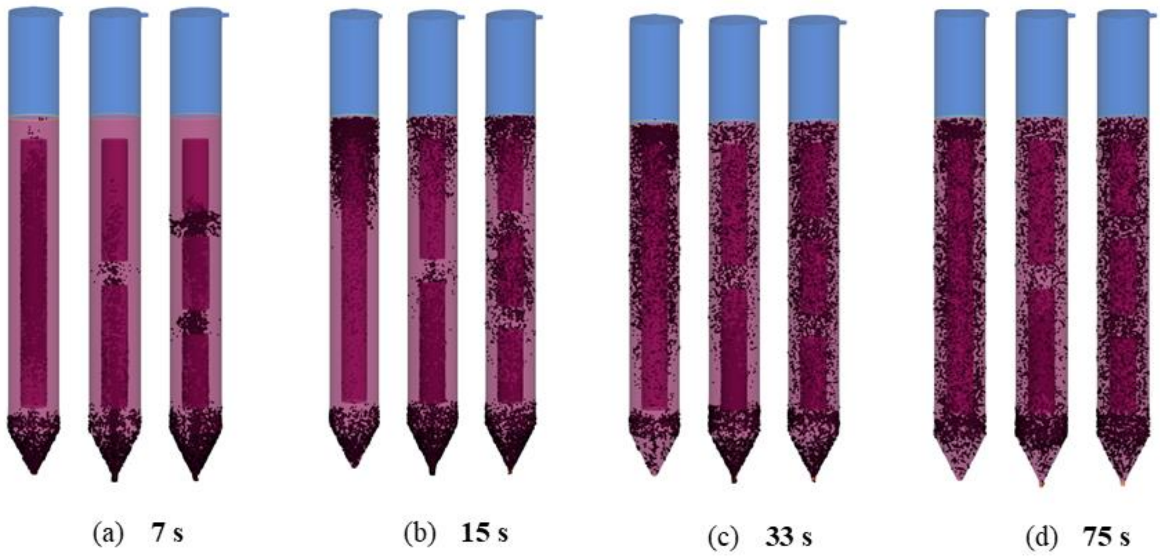


Figure 41. Lagrangian particles coupled with the liquid phase (a) at 7 seconds, (b) at 15 seconds, (c) at 33 seconds, and (d) at 75 seconds. Adapted from **Conference Publication 1**.

Figure 42 depicts the trajectories of 25 particles over a 75-second simulation, with the color's bar representing a maximum velocity limit of 0.2 m/s. The circulation loop on the top draft tube in the double-stage geometry (DDG) is visible, while none of the observed particles exhibit the second circulation loop. On the contrary, in the triple-stage geometry (TDG), all three circulation loops are observed among the 25 particles.

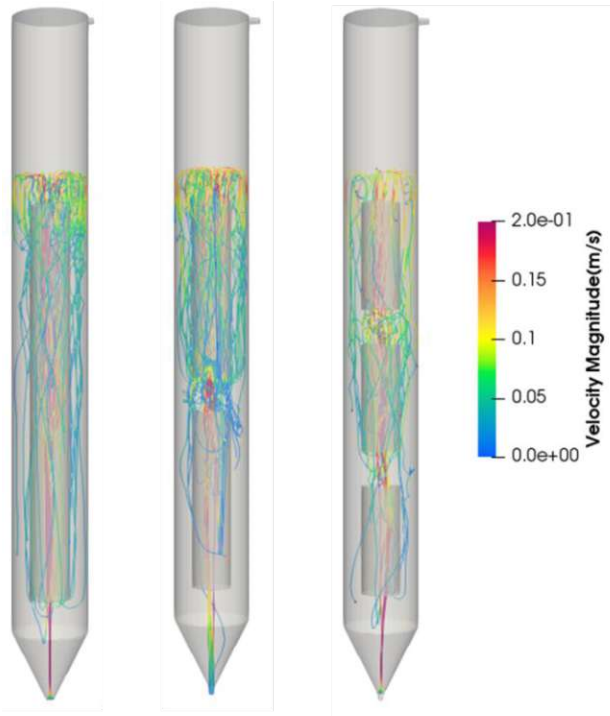


Figure 42. Particle tracks of 25 particles with particle velocity magnitude (m/s) during 75 seconds of simulation. Adopted from **Conference Publication 1**.

5.4. Power consumption in continuously stirred tank reactors

Continuing with exploring different bioreactors that play a crucial role in the bioeconomy, CSTRs emerge as another widely utilized option. In contrast to air lift bioreactors, which were the focus of the previous hydrodynamic study, CSTRs offer their own unique characteristics and operational considerations. One important aspect that requires careful examination in CSTRs is power consumption, which can significantly impact the overall efficiency and cost-effectiveness of the bioprocess. To quantify and analyze power consumption in CSTRs, the concept of the Power Number becomes a fundamental parameter to investigate.

As mentioned in the research approach, this study involved experiments and simulations of three types of stirrers: pitched blade, cage, and paddle. Throughout the experimental phase, the velocity was incrementally augmented until the occurrence of unstable vibrations, which impeded the torque measurement. To obtain comprehensive data, torque measurements were documented for each type of stirrer within predefined ranges of rotational speeds in revolutions per minute (RPM): stirrer 1 ranged from 550 to 1300 RPM, stirrer 2 ranged from 400 to 950 RPM, and stirrer 3 ranged from 130 to 325 RPM.

The torque outcomes from the experimental investigation and simulation scenarios for three distinct stirrers are presented in Table 14. In the case of Stirrer 1 and Stirrer 2, the experimental torque demonstrates a progressive increase as the rotational speed escalates. On the other hand, for Stirrer 3, the experimental torque consistently exceeds the simulated torque in all cases. The largest disparity between the experimental and simulated torque values is observed for Stirrer 3 at higher rotational speeds. One plausible explanation for these inconsistencies is that the experimental equipment employed is primarily designed for instructional purposes and has not undergone calibration since its installation.

Table 14. Comparison of experimentally measured vs. simulated torque.

	Stirrer 1			Stirrer 2			Stirrer 3	
Case	Experimental ($x10^{-2}$ Nm)	Simulated ($x10^{-2}$ Nm)	Case	Experimental ($x10^{-2}$ Nm)	Simulated ($x10^{-2}$ Nm)	Case	Experimental ($x10^{-2}$ Nm)	Simulated ($x10^{-3}$ Nm)
550	1	5.59	400	2	2.11	130	2	3.03
650	6	7.84	500	11	3.30	150	11	4.06
750	11	10.45	600	17	4.75	175	17	5.55
850	15	13.37	700	24	6.42	200	23	7.24
950	19	16.70	800	31	8.42	250	39	11.23
1050	26	20.33	850	35	9.57	275	47	13.50
1150	30	24.36	900	40	10.76	300	57	16.06
1250	36	28.83	950	44	11.92	325	67	18.85

Table 15 compares the power numbers obtained from experimental measurements and CFD simulations for the three different stirrers. In the case of Stirrer 1, the experimental power number gradually increases with higher rotational speeds (cases). Conversely, the simulated power number remains relatively consistent at approximately 5.26 across all cases. Stirrer 2 exhibits a noticeable deviation between the experimental and simulated power numbers. At lower rotational speeds (cases 400-500), the experimental power number significantly surpasses the simulated power number. Stirrer 3 demonstrates significantly higher experimental power numbers than the simulated ones, particularly at higher rotational speeds. These findings suggest potential inaccuracies in the predictions of the CFD simulations or discrepancies arising from the lack of calibration for the laboratory stirrer controller, IKA EUROSTAR 200.

Table 15: Comparison of experimentally measured vs. simulated power number.

	Stirrer 1			Stirrer 2			Stirrer 3	
Case	Experimental	Simulated	Case	Experimental	Simulated	Case	Experimental	Simulated
550	0.94	5.26	400	66.74	70.24	130	33.73	5.12
650	4.05	5.29	500	234.92	70.44	150	139.34	5.15
750	5.57	5.30	600	252.12	70.51	175	158.22	5.17
850	5.92	5.28	700	261.51	69.96	200	163.89	5.16
950	6.00	5.27	800	258.61	70.22	250	177.85	5.12
1050	6.72	5.26	850	258.64	70.70	275	177.13	5.09
1150	6.47	5.25	900	263.66	70.89	300	180.51	5.09
1250	6.57	5.26	950	260.30	70.49	325	180.80	5.09

Figure 43 shows the flow pattern of the stirrers and the velocity profiles of the CSTRs colored at a maximum velocity magnitude of 2.6 m/s for the case of the pitched blade (a) and the cage impeller (b) and colored at a maximum velocity magnitude of 1.3 m/s for the case of the paddle impeller (c). For the pitched blade impeller, the case of 750 RPM was used; for the cage impeller, the case of 700 RPM was chosen; for the paddle impeller, the case of 300 RPM was selected for this figure.

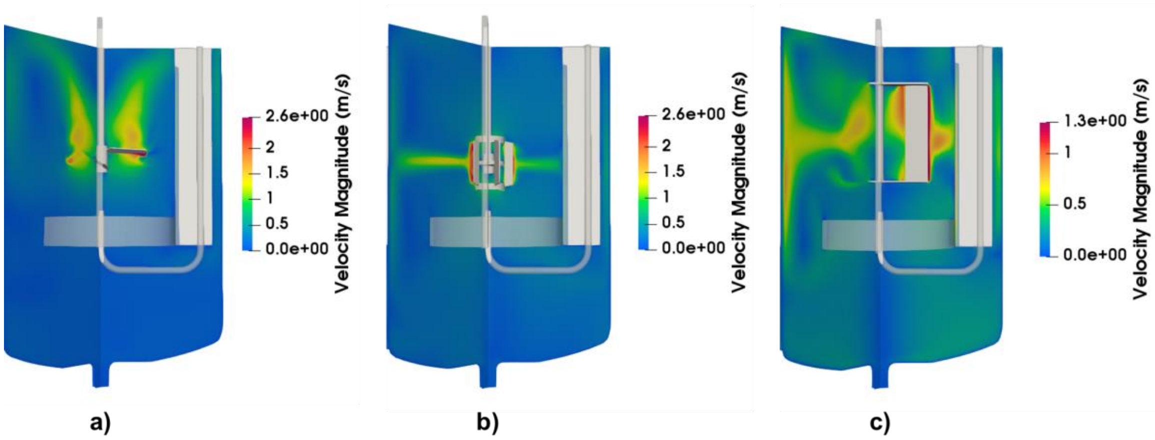


Figure 43. Velocity profiles of three stirrer types a) pitched blade at 750 RPM, b) 6-cage impeller at 700 RPM, and c) paddle impeller at 300 RPM. Adopted from **Journal Publication 5**.

The subsequent section depicts 8 cases for each stirrer geometry, with the velocity magnitude illustrated through color. Figure 44 displays the velocity profiles of Stirrer 1, highlighting the maximum velocity magnitude at 2.6 m/s. Similarly, Figure 45 exhibits the velocity profiles of Stirrer 1, with the maximum velocity magnitude colored at 1.2 m/s. Furthermore, Figure 46 showcases the velocity profiles of Stirrer 1, emphasizing the maximum velocity magnitude at 0.75 m/s.

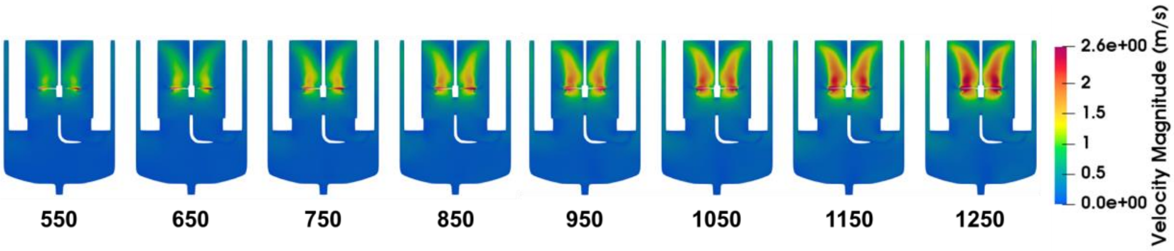


Figure 44. Velocity profiles stirrer 1 at 550, 650, 750, 850, 950, 1050, 1150, and 1250 RPM. Adopted from **Journal Publication 5**.

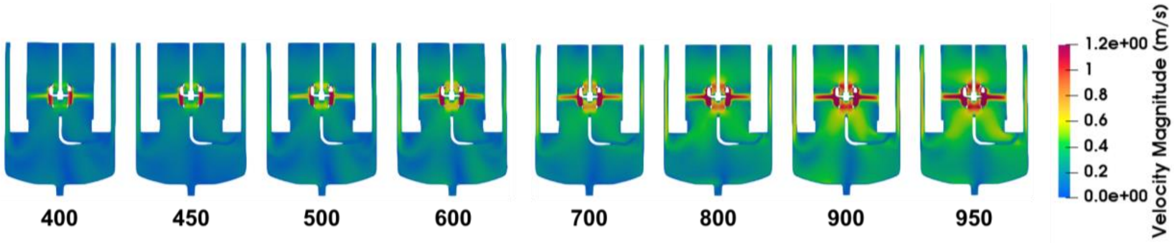


Figure 45. Velocity profiles stirrer 2 at 400, 450, 500, 600, 700, 800, 900, and 950 RPM. Adopted from **Journal Publication 5**.

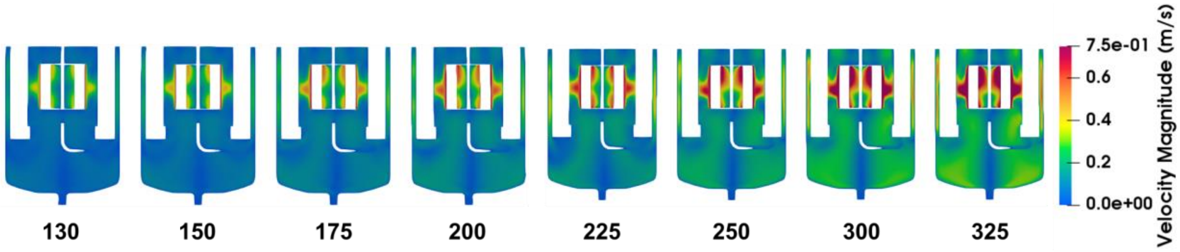


Figure 46. Velocity profiles stirrer 3 at 130, 150, 175, 200, 225, 250, 300, and 325 RPM. Adopted from **Journal Publication 5**.

5.5. Retrofitting existing infrastructure for the bioeconomy

Journal Publication 6 aims to shift the existing paradigm of slurry disposal systems in Ireland, which currently contributes to ozone layer depletion and methane emissions from animal manures, such as cow and pig manure. These emissions have a significant global warming potential since each molecule of methane has a greater potential (25 times more over 100 years) for contributing to global warming compared to a carbon dioxide molecule; its capture and utilization as a fuel can offer one of the most environmentally friendly energy sources available (Abbasi et al., 2011). However, the high cost of farm-scale anaerobic digesters makes them financially unviable for many farmers, leading to the utilization of ELS tanks or slurry tower tanks for manure storage.

In contrast, the proposed system presented in **Journal Publication 6** offers an innovative and cost-effective solution. The system provides several benefits by collecting the slurry from the barns and channelling it into a covered lagoon. Firstly, the biogas generated from the slurry can be harnessed for the production of electricity and/or heat, offering an alternative energy source. This reduces harmful emissions and creates potential revenue streams through the sale of excess biogas. Moreover, the produced heat can be utilized to warm the covered lagoon, ensuring optimal anaerobic digestion conditions. Additionally, the electricity generated can be used to power the barn or dairy plant, promoting energy efficiency.

Furthermore, the system allows for the safe utilization of the digestate, the liquid-solid fraction remaining after digestion, as a nutrient-rich fertilizer for fields. This closed-loop approach minimizes waste and promotes sustainable agricultural practices. Figure 47 illustrates the proposed system's transition from the current environmentally damaging approach to an environmentally friendly and economically viable system. With its lower cost and scalability, the proposed system in **Journal Publication 6** offers a promising alternative for slurry disposal, addressing environmental concerns while providing economic benefits for farmers.

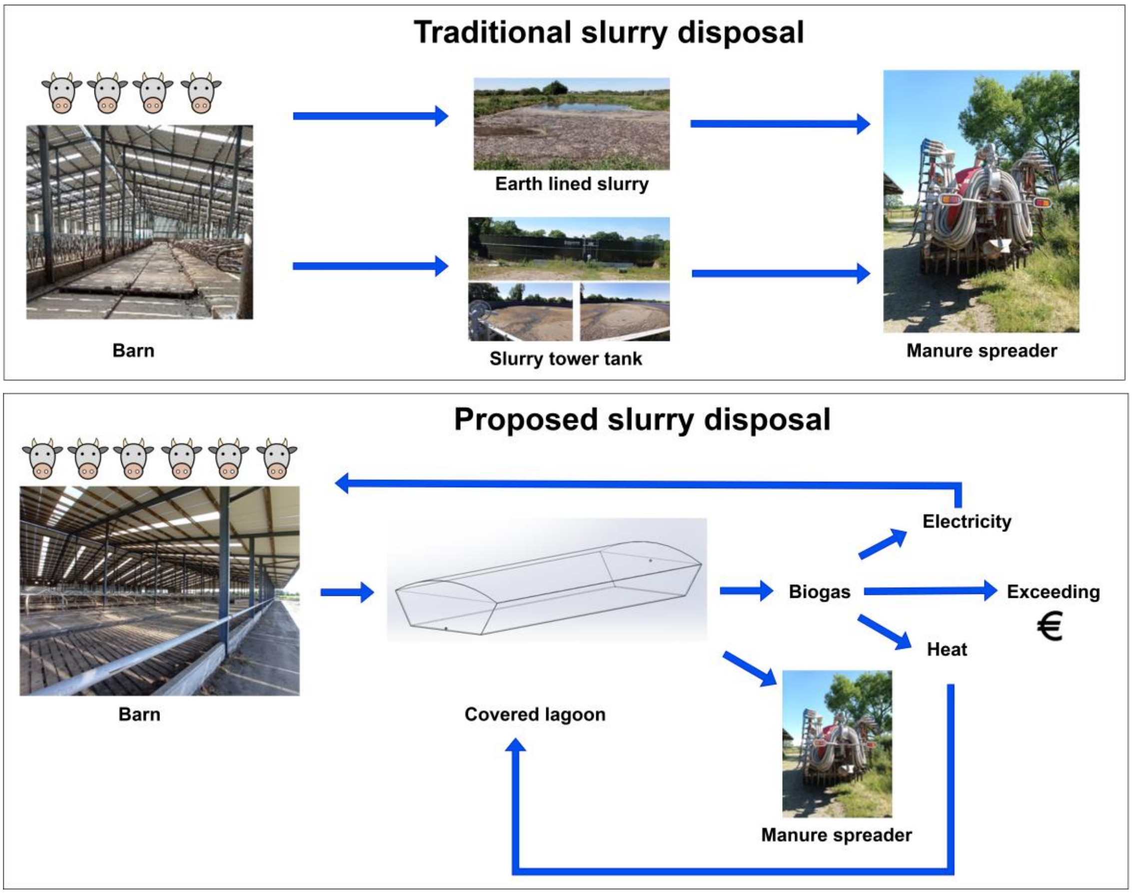


Figure 47. Proposed systematic transition.

As described in the research approach, the attributes associated with the system's configuration were evaluated from 0 to 10, where zero indicates poor performance, and ten indicates outstanding performance. The evaluation considered seven attributes: performance, economic viability, efficiency, reliability, scalability, ecological sustainability, and environmental risks. Performance refers to the effectiveness and efficiency of the system in achieving its intended outcome, and it assesses how well the system performs its designated functions and meets established performance criteria. Efficiency measures the extent to which the system minimizes waste, conserves energy, and maximizes output. Efficiency aims to achieve the desired objectives with minimal resource inputs. Reliability refers to the ability of the system to perform its intended functions without failures or disruptions consistently, and also refers to robustness and ability to deliver consistent and predictable results over time. Scalability assesses the capacity of the system to adapt, expand, and reduce its volume. Ecological sustainability evaluates the environmental impacts of the system throughout its life cycle. Environmental risks refer to the potential for adverse environmental impacts if the system is not managed correctly. Economic viability evaluates the financial feasibility of the system by assessing capital costs. The spider graph in Figure 48 evaluates the three system configurations proposed.

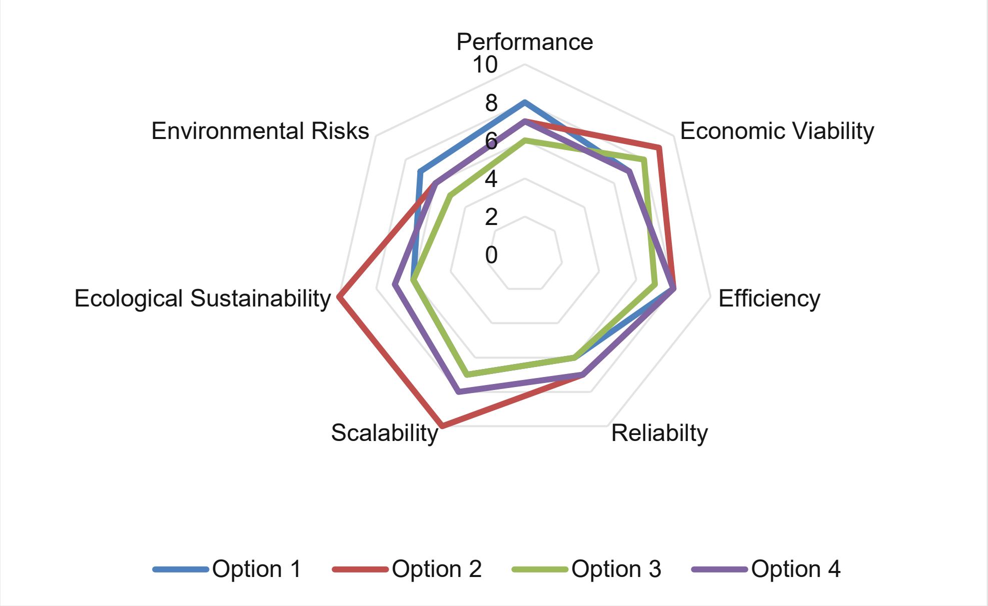


Figure 48. Attribute evaluation of different proposed configurations.

The model is not considering pasteurization of the feedstock. The manure is pulled with the scrappers to be sent to a pretreatment tank, where water is added to get a ratio of 2:1 (water to manure) and heated up. From this pretreatment tank, the slurry is then sent to a plug flow reactor where the hydrolysis and acidogenesis take place; the hydraulic retention time of the slurry is 8 to 10 days. The slurry then passes to the covered lagoon, where it takes another 17-20 days to have the acetogenesis and methanogenesis steps. From the covered lagoon the digestate is dewatered and passed to an ELS tank to be then spread in the fields. The unutilized digestate is sold as organic fertilizer, generating extra income for the farm. Figure 49 shows a schematic representation of the process that was just described above.

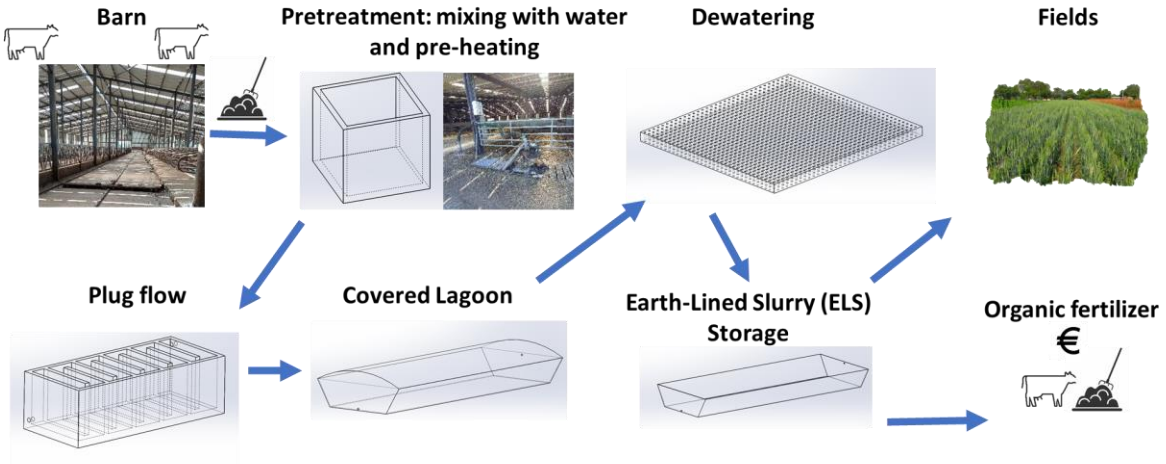


Figure 49. Schematic of the proposed system.

Figure 50 shows a schematic of the heating system. The streams of water and biogas are shown with green arrows for water and yellow for the biogas. First, the biogas is extracted from the covered lagoon and passes to a biogas storage bag made from a polyethylene membrane. Then it passes through a desulphurization process to be burned in a boiler (shown with yellow arrows). The biogas boiler heats water and passes it first through the covered lagoon where the temperature needed is 38 ºC. The water piping system then passes through the first stage of the digestion process (the plug flow reactor), finally through the pretreatment section, and then recycled to the boiler. Figure 50 shows the water (green arrows) and biogas (yellow arrows) streams of the system.

A desulphurization method is needed to remove the hydrogen sulfide (H_2S) from the raw biogas. Typical methods are biological scrubbers, which convert the H_2S utilizing biological conversion to elemental sulfur and sulfate; sulfide precipitation by using liquid metal salts such as iron hydroxide or iron chloride; or adsorption of activated carbon, copper oxide, zinc oxide, or iron oxide (Miltner et al., 2012). A fourth method was developed by Miltner et al. (2012), which is a chemical-oxidative scrubbing method for the biomethane plant in Bruck an der Leitha.

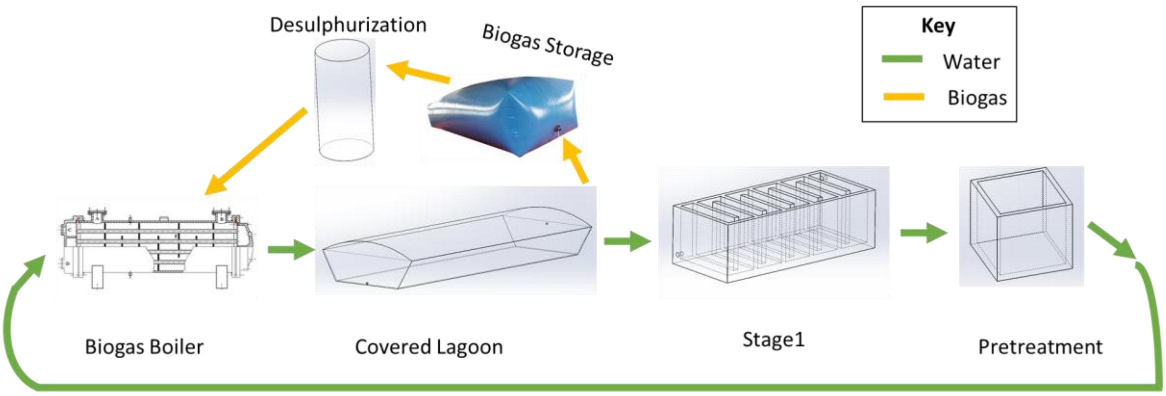


Figure 50. Water and biogas streams in the system.

When burning the biogas, it must be considered that the boiler's efficiency plays a critical role. The average calorific value of biogas ranges from 21-23.5 MJ/m³, equating to approximately 0.5-0.6 liters of diesel fuel or an energy content of around 6 kWh, although conversion losses limit its conversion to only about 1.7 kWh_{el} per 1 m³ of biogas (Energypedia, 2016).

The retrofitting solution presented in **Journal Publication 6** offers a promising and sustainable alternative for slurry disposal. By collecting and channeling slurry into a covered lagoon, the system enables biogas generation for electricity and heat production, reducing harmful emissions and creating potential revenue streams. Safely utilizing digestate as fertilizer promotes closed-loop agricultural practices, minimizing waste and environmental impact. With its cost-effectiveness and scalability, the proposed system addresses environmental concerns while providing economic benefits for farmers. Overall, this innovative solution represents a significant step towards a more sustainable and environmentally friendly approach to slurry management.

5.6. Safety considerations in biorefinery design and operation

The safe by design framework represents a comprehensive approach to ensure biorefinery operations' safety, environmental responsibility, and reliability. It encompasses various stages and interconnected elements that work together to minimize risks, protect the environment, and promote secure and sustainable practices.

Figure 51 illustrates an integrated framework for safe by design in biorefineries. The central circle represents the biorefinery system, while eight outer circles represent key elements of the framework. The figure emphasizes the interconnectedness and interdependence of these elements in ensuring the safety and reliability of biorefinery operations. The framework encompasses various stages, starting with hazard identification, where potential risks associated with biorefinery processes are thoroughly assessed. Risk and reliability assessment evaluates the likelihood and severity of identified hazards, while design integration integrates safety considerations into the early stages of biorefinery design. Inherent safety principles aim to minimize hazards at their source, and control measures are implemented to mitigate risks. Monitoring, maintenance, and reliability management ensure ongoing safety and performance, while emergency preparedness addresses potential incidents or accidents. Compliance and auditing ensure adherence to safety protocols, and the framework promotes continuous improvement through communication, training, and total quality management. The figure visually represents the comprehensive approach to safe by design, highlighting the importance of integrating safety measures across all aspects of biorefinery operations.

Figure 51. Integrated Framework for Safe by Design in Biorefineries.

Figure 52 represents the comprehensive framework for safe by design in biorefineries, visualized as an onion with layers. At the center of the figure, we find the human element, symbolizing the utmost importance of ensuring the safety and well-being of workers and surrounding communities throughout the biorefinery processes. Moving outward, the second layer focuses on implementing robust safety measures in biotechnology to prevent the release of genetically modified organisms and microorganisms outside the facility. The third layer emphasizes the need to maintain the integrity of feedstock materials and avoid cross-contamination along the production processes. The fourth layer highlights the significance of environmental considerations, promoting practices that minimize the environmental impact of biorefinery operations. Lastly, the outermost layer represents the reliability of processes, emphasizing the importance of robust design, quality control, and regular maintenance to ensure consistent and predictable performance. Together, these layered elements form a holistic framework that prioritizes safety, environmental responsibility, and reliability in the design and operation of biorefineries, promoting secure and sustainable practices in this important field.

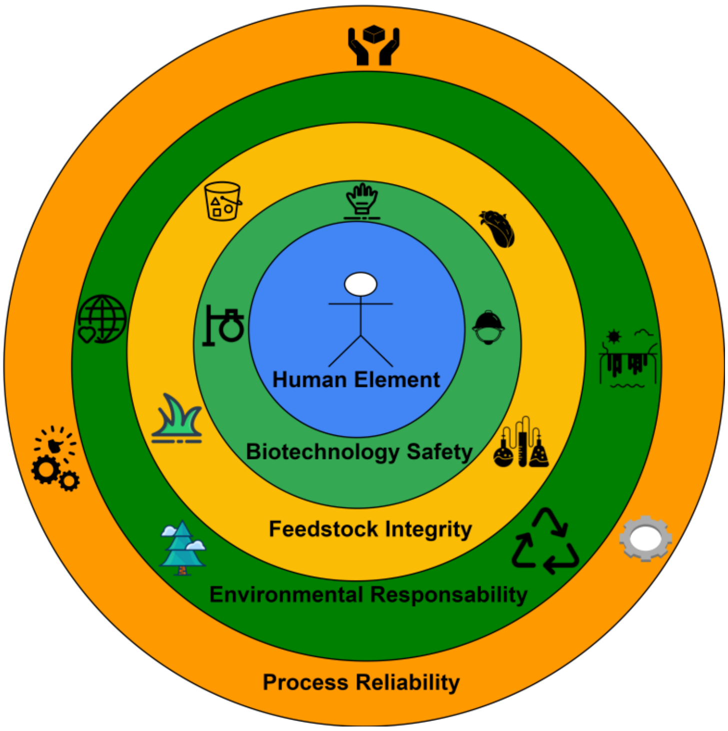


Figure 52. Comprehensive Framework for Safe by Design in Biorefineries: Layered Approach for Safety, Environmental Responsibility, and Reliability.

5.7. Summary

This thesis involved multidisciplinary works with a significant focus on CFD, but also in other areas, such as systems design, such as the case of **Journal Publications 1, 6, and 7**, and case studies, such as the case of **Journal Publications 1 and 2**. Other topics in this thesis include deep research in the state of the art in biorefineries and biogas plants (**Public Report 2**), the development of an opensource toolbox for the investigation of bioreactors (**Public Report 3**), the investigation of a novel feedstock for anaerobic co-digestion with animal manures proposed in **Conference Poster 2**.

One of the main lines of research was air lift reactors, from research, computational experimentation with CFD, dissemination in publications, to presentations as posters and oral presentations. A detailed description of this line of research is presented as a timeline in Figure 22.

Another line of research was developed from proof of concept in **Conference Poster 1**, where the idea was presented to the scientific community at the Circular@WUR conference. Due to the acceptance and feedback of this model, **Journal Publication 1** was developed. Once **Journal Publication 1** had been published, this work was presented by Cabrera-Gonzalez (2022) in the Bioeconomy Research Symposium: Ireland 2022 celebrated in Dublin, Ireland, and by Ramonet (2022) as a keynote presentation titled Circular Bioeconomy Applications (Spanish: “Aplicaciones de la Economia Circular”) in the 1st International Congress of "Environmental Biotechnology and Circular Economy (Spanish: “I Congreso Internacional de “Biotecnología Ambiental y Economía Circular”) in Lima, Peru.

Furthermore, the importance of multidisciplinary research cannot be overstated in the context of addressing complex challenges in the field of anaerobic digestion. Integrating diverse disciplines, such as CFD, systems design, biorefineries, and biogas plants, allows for a holistic and comprehensive approach to tackling the complexities of anaerobic digestion systems. CFD was utilized to explore not-so-well-studied systems, such as the multi-stage internal loop air lift reactor. From where insight on how the draft tubes configuration and morphology affects the overall hydrodynamics of these systems. Utilizing the systems approach, the synergetic integration of state-of-the-art technologies was performed in the circular economy model for desert coastal regions. Thinking with a more holistic approach, unutilized carbon dioxide was proposed for greenhouse crop farming, and the proposition of retrofitting and building anaerobic covered lagoons as a solution to the problem of scale faced by the Irish farmers in their manure management systems. By combining knowledge and tools from various fields, researchers can explore different dimensions of the problem, leading to innovative solutions and a deeper understanding of the underlying processes.

Multidisciplinary research facilitates the exchange of knowledge, methodologies, and perspectives, promoting collaboration among experts with diverse backgrounds. In this thesis, the fusion of CFD with systems design provides a powerful tool to optimize the performance and efficiency of anaerobic digestion and biorefinery systems. The insights gained from studying biorefineries and biogas plants contribute to developing sustainable and environmentally friendly practices in waste management and renewable energy production.

Chapter 6. Conclusions and Outlook

In conclusion, this thesis has dug into circular bioeconomy in chemical engineering, employing a multidisciplinary research approach to explore various aspects of resource utilization, waste management, and sustainable practices. Through theoretical analysis, CFD simulations, case studies, data analysis, and conceptual modeling, valuable insights have been gained, leading to the development of innovative solutions and the evaluation of their potential impact.

The findings of this thesis highlight the importance of adopting a circular bioeconomy model for desert coastal regions, where resource scarcity and environmental challenges pose significant obstacles. By leveraging CO_2 utilization for greenhouse crop farming, the potential for sustainable agricultural practices is expanded, promoting resource efficiency and reducing carbon emissions. Furthermore, the application of CFD in air lift bioreactors and continuously stirred tank reactors has provided crucial insights into optimizing the design and operation of these systems, enhancing their productivity and economic viability.

Another significant contribution of this thesis is the proposal of retrofitting slurry tanks into covered lagoons, offering a promising solution to the scale issue faced by anaerobic digesters and addressing the challenges of Irish farmers in slurry disposal. This innovative approach mitigates environmental concerns related to ozone depletion and methane emissions and brings economic benefits through utilizing biogas for electricity and heat production. Additionally, the development of a safe-by-design framework for biorefineries emphasizes the importance of integrating safety considerations from the conceptual design phase, ensuring secure and sustainable operations.

In summary, the multidisciplinary nature of this thesis has enabled a comprehensive exploration of anaerobic digestion systems and their potential for sustainable biorefinery applications. The integration of CFD, systems design, and the study of biorefineries and biogas plants has yielded valuable insights and innovative solutions for waste management and renewable energy production. However, further research is needed to identify and propose retrofitting existing industrial infrastructure into biorefinery systems, considering scalability, economic feasibility, and environmental impact. By continuing to bridge the gaps between different disciplines and leveraging their collective knowledge and tools, we can unlock the full potential of anaerobic digestion as a key component of the circular economy. Looking ahead, ongoing research and development in the field of circular bioeconomy in chemical engineering, including the exploration of advanced technologies such as CFD applied to biotechnology, will contribute to the development of more efficient processes. Moreover, collaborations between academia, industry, and policymakers will play a vital role in implementing and scaling up circular bioeconomy initiatives, fostering a successful transition toward a more sustainable and environmentally friendly future.

In conclusion, this thesis has provided valuable insights into the potential and obstacles of the circular bioeconomy in chemical engineering. The research conducted in this study lays the groundwork for future progress in sustainable resource management, waste reduction, and the integration of circular principles into industrial processes. By embracing these principles and fostering ongoing innovation, we can work towards creating a more sustainable and resilient society. This involves a balanced approach where economic growth is harmonized with environmental stewardship, ensuring a prosperous future for both current and future generations.

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Appendix A

List of publications

Journal publications

- Cabrera-González, M.; Ramonet, F.; Harasek, M. Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions. Land 2022, 11, 1506. https://doi.org/10.3390/land11091506
- Ramonet F., Jordan C., Haddadi B., Harasek M., (2022), Anaerobic Digestion as a Carbon Capture, Storage, and Utilization Technology, Chemical Engineering Transactions, 96, 49-54. https://doi.org/10.3303/CET2296009
- Ramonet, F., Haddadi, B., Jordan, C., Harasek, M. (2022). Modelling and Design of Optimal Internal Loop Air-Lift Reactor Configurations Through Computational Fluid Dynamics. Chemical Engineering Transactions, 94, 817-822. https://doi.org/10.3303/CET2294136
- Ramonet, F., Haddadi, B., & Harasek, M. (2023). Optimal Design of Double Stage Internal Loop Air-Lift Bioreactor. Energies, 16(7), 3267. https://doi.org/10.3390/en16073267
- Ramonet F., Haddadi B., Kovacevi, M., Jordan C., Harasek M. (2023), Bioreactor Mixing: A Comparison of Computational Fluid Dynamics and Experimental Approaches in the Pursuit of Sustainable Bioprocessing for the Bioeconomy**.** Submitted to Chemical Engineering Transactions.
- Ramonet, F., Gleeson, T., Galvin, M., Haddadi, B, Harasek, M., (2023), Anaerobic Digestion as A Tool to Mitigate Greenhouse Gas Emissions from Animal Slurries. Unpublished manuscript.
- Ramonet, F. Cabrera-González, M., Harasek, M. Promoting Safe Operations in Biorefineries: A Comprehensive Safe by Design Framework. Manuscript in writing.

Conference publications

- Ramonet, F., Haddadi, B, Harasek, M., (2023), Modelling of Multi-Stage Internal Loop Air Lift Bioreactor Utilizing Computational Fluid Dynamics, 7th Minisymposium Verfahrenstechnik and 8th Partikelforum, BOKU, Vienna, April 13th – 14th, ISBN: 978-3-900397-08-1. Avaialable: http://www.chemical-engineering.at/minisymposium/assets/Tagungsband_miniVT_2023.pdf
- Mayuki Cabrera-González, Fernando Ramonet, Michael Harasek. Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions. Circular@WUR: Living within planetary boundaries, Wageningen University and Research, Wageningen, 11-13 April, 2022. DOI: 10.13140/RG.2.2.21658.11200

- Fernando Ramonet, Michael Harasek. Modelling Study on the Co-Digestion of Nopal Cladodes with Farm Manures. 30th European Biomass Conference & Exhibition (EUBCE2022).Paris, France (online), 9-12 May, 2022, ISBN: 978-88-89407-22-6
- Fernando Ramonet, Bahram Haddadi, Michael Harasek. Modelling And Characterization Of Internal Loop Air Lift Bioreactor Configurations Through Computational Fluid Dynamics. Biorefine Conference 'The role of biorefineries in European agriculture'. Ghent, Belgium, 30-31 May, 2022. DOI: 10.13140/RG.2.2.16383.89765

Public reports

- Balachandran, Srija; Cerca, Mariana; Chopda, Rushab; Ramonet, Fernando; Vance, Charlene; De Meester, Steven; Harasek, Michael; Meers, Erik; Murphy, Fionnuala; Robles-Aguilar, Ana. (2021). State-of-the-art Report on Anaerobic Digestion and Biorefinery Systems Level Design. European Comission. Reference Ares(2021)2235935 - 31/03/2021. https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5db4cee55&appId=PPGMS
- Ramonet, Fernando; Harasek, Michael. CFD optimisation and analysis of existing AD and Biorefineries Report. Reference Ares(2021)7353824 - 29/11/2021. https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5e52d5093&appId=PPGMS
- Ramonet, Fernando; Harasek, Michael. Geometry and CFD results for AD retrofit and TPB up scaling Report. Submitted 7 February 2023.

Journal Publication 1

Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions

published in Land in collaboration with Mayuki Cabrera-González and Michael Harasek.

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Cabrera-González, M.; Ramonet, F.; Harasek, M. Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions. Land 2022, 11, 1506. https://doi.org/10.3390/land11091506

Journal Publication 2

Anaerobic Digestion as a Carbon Capture, Storage, and Utilization Technology

published in Chemical Engineering Transactions in collaboration with Christian Jordan, Bahram Haddadi and, Michael Harasek.

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Ramonet F., Jordan C., Haddadi B., Harasek M., (2022), Anaerobic Digestion as a Carbon Capture, Storage, and Utilization Technology, Chemical Engineering Transactions, 96, 49-54. https://doi.org/10.3303/CET2296009

Journal Publication 3

Modelling and Design of Optimal Internal Loop Air-Lift Reactor Configurations Through Computational Fluid Dynamics

published in Chemical Engineering Transactions in collaboration with Bahram Haddadi, Christian Jordan and, Michael Harasek.

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Ramonet, F., Haddadi, B., Jordan, C., Harasek, M. (2022). Modelling and Design of Optimal Internal Loop Air-Lift Reactor Configurations Through Computational Fluid Dynamics. Chemical Engineering Transactions, 94, 817-822. https://doi.org/10.3303/CET2294136

Journal Publication 4

Optimal Design of Double Stage Internal Loop Air-Lift Bioreactor

published in Energies in collaboration with Bahram Haddadi and, Michael Harasek.

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Ramonet, F., Haddadi, B., & Harasek, M. (2023). Optimal Design of Double Stage Internal Loop Air-Lift Bioreactor. Energies, 16(7), 3267. https://doi.org/10.3390/en16073267

Journal Publication 5

Bioreactor Mixing: A Comparison of Computational Fluid Dynamics and Experimental Approaches in the Pursuit of Sustainable Bioprocessing for the Bioeconomy

submitted to Chemical Engineering Transactions in collaboration with Mara Kovacevic, Bahram Haddadi, Christian Jordan and, Michael Harasek.

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Journal Publication 6

Anaerobic Digestion as A Tool to Mitigate Greenhouse Gas Emissions from Animal Slurries

Collaboration with Tim Gleeson, Micheal Galvin, Bahram Haddadi, and Michael Harasek

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Status: in writing

ANAEROBIC DIGESTION AS A TOOL TO MITIGATE GREENHOUSE GAS EMISSIONS FROM ANIMAL SLURRIES

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Abstract

Anaerobic Digestion (AD) has been gaining popularity in the last decades for the production of biogas from organic waste, agricultural waste, and energy crops. Biogas is a mixture of approximately 70 % methane, 29 % carbon dioxide, and 1 % other gases. Biogas plants produce electrical and thermal energy by burning the biogas in combined heat and power units or upgrade the biogas into a 95 % to 99 % pure biomethane, which can then be injected into the grid or used as a transport fuel. A wet mixture called digestate is left after biogas production. The digestate is a great fertiliser since it contains all nutrients and micronutrients for needed for agriculture such as potassium, phosphorus, and nitrogen. Ireland is distinguished by the European Commission as the country with the largest biomethane potential in Europe. The Irish Biogas Association states that biogas produced using AD technology should be at the core of Ireland's future energy mix. In Ireland, the animal slurry is currently being stored in open tanks, emitting greenhouse gas emissions. Each particle of methane is 25 times more harmful than a particle of carbon dioxide. By 2022, Ireland's livestock includes more than 7 million cows, 1.7 million pigs, and 16.5 million poultry per year. In this study, we propose modelling the retrofitting of existing open slurry tanks into covered lagoons to harvest the biogas from the animal slurries to reduce greenhouse emissions. The digestate will be utilised as fertiliser to enhance soil health, crop yield, and productivity. Based on average herd sizes and daily slurry availability, optimal covered lagoon dimensions will be found. A global value will be obtained for the biogas potential from animal slurries in Ireland.

1. Introduction

The emission of greenhouse gases is dominated by carbon dioxide (74 %), followed by methane (17 %), nitrous oxide (6.3 %), and fluorinated gases (2.3 %), which possess a high global warming potential (WRI, 2021). Although each methane molecule has a higher global warming potential than a molecule of carbon dioxide, utilizing captured methane as a fuel can lead to one of the cleanest energy sources (Abbasi et al., 2011).
The agricultural sector is recognized as a challenging area for emissions reduction due to the difficulty in mitigating methane emissions from enteric fermentation and the problems associated with open tank manure storage, including fugitive methane emissions, eutrophication, and groundwater contamination in wet climates (Diaz Huerta et al., 2023). The removal of manure from animal houses has been shown to significantly reduce CH_4 emissions, resulting in a decrease ranging from 50 % to 60 % (Scott and Blanchard, 2021).
The increasing recognition of climate change consequences is driving pressure on the Irish government to mitigate environmental impact, with anaerobic digestion (AD) emerging as a promising technology in the agriculture sector for its potential to generate renewable energy, reduce GHG emissions, and promote a circular economy (O'Connor et al., 2023). By the end of 2022, Ireland's livestock includes more than 6.55 million cows, 1.57 million pigs, and 16.5 million poultry per year (CSO, 2022).
According to the TEAGASC National Farm Survey, the average dairy farm in Ireland grew from a herd size of 64 in 2012 to 93 in 2022 (TEAGASC, 2023).
Researchers aim to mitigate the environmental impacts related to manure management in dairy farms through the proposal of utilizing biogas production as an alternative solution (Rivas-Garcia et al., 2015).
Manure is typically stored in open ponds or storage tanks until it is time for spreading on the fields. The degradation process of animal manure involves a series of interconnected microbial steps, in an uncovered anaerobic lagoon the treatment follows a general pattern illustrated in **Figure 53**. Settleable solids from the manure settle at the lagoon's bottom, where they break down into sludge, liquids, and gases. Soluble organic matter enters the treatment process at specific stages. Lagoons have various microbial communities that work together symbiotically to digest organic material. The extent of organic matter degradation is influenced by the

composition of these communities and the characteristics of the influent. These lagoon microbial communities encompass anaerobic and facultative heterotrophic bacteria, phototrophic organisms, and aerobic bacteria.

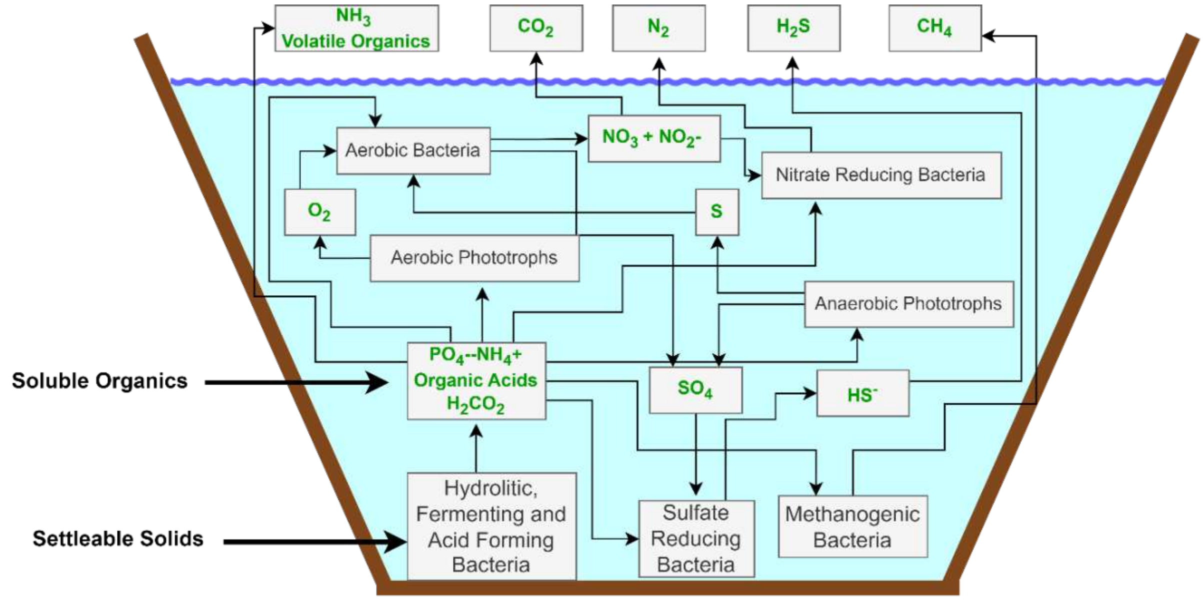

Figure 53. Biological degradation of manure in uncovered anaerobic lagoons. Adapted from (Hamilton et al., 2006).

Ireland is lacking behind the rest of the European Union with approximately 20 AD plants (IrBEA, 2023). According to the Irish Bioenergy Association's (IrBEA) Statement on Biomethane to the Oireachtas Joint Committee on Agriculture, Food, and the Marine (IrBEA, 2023), anaerobic digestion (AD) can be effectively employed at a farm scale to manage slurry and farmyard manure. This process enables the efficient recycling of valuable nutrients and the recovery of energy for on-farm use, while also reducing ammonia emissions and improving nutrient availability. By implementing on-farm digestion, farms can effectively decarbonize their operations while sustaining food production activities. This approach involves the early-stage utilization of slurry in AD, allowing for optimal methane capture for energy generation and minimizing emissions.
The limited adoption of anaerobic digestion (AD) technology in Ireland can be attributed to the emphasis on larger farms that have the financial means to implement such technology, as well as the higher occurrence of summer pasture grazing practices (Scott and Blanchard, 2021).
The low adoption rate of this technology in Ireland, in comparison to other European countries, can primarily be attributed to the level of uncertainty it presents to farmers in terms of financial returns (Diaz Huerta et al., 2023). According to O'Connor et al. (2020), medium and large-scale biogas plants in Ireland are not feasible since the average Irish dairy farm has 90 cows (2018), which does not provide enough feedstock for the digesters.
An example of the utilization of biogas from farm-scale anaerobic digestion was proposed by Scott and Blanchard (2021). Their recommendation involves the integration of combined heat and power (CHP) units within the digesters to effectively utilize the generated heat and electricity. First using the electricity to power the stirrers and the heat to warmth the reactor. The surplus electricity can be utilized for a range of farm activities, such as powering milking machines, facilitating milk cooling, operating the scraping system, and providing adequate lighting. Additionally, the excess heat can be used to fulfil the heating requirements of the farm. Furthermore, the authors suggest utilizing a fraction of the produced methane as a valuable fuel source for powering tractors, road vehicles, and other agricultural machinery. By implementing these strategies, the overall energy potential of the digesters can be maximized, contributing to the sustainable and efficient operation of small-scale farm-based anaerobic digestion systems.
To maximize the potential deployment of small-scale anaerobic digestion (SSAD) plants and attract investors, it is crucial for government support programs to recognize the additional costs associated with smaller capacity facilities and implement policies that offset these expenses. Despite the demonstrated viability of SSAD plants, substantial government support is required to achieve financial returns that are appealing to potential investors (O'Connor et al., 2020).
In 2022, during the Energy and Farm Business show, the Minister of Agriculture announced that in the next months grants would be made available for farm anaerobic digestion. This was followed by a press release announcing a 12-million-euro investment in the next four years (McConalogue, 2022). In the first year,

McConalogue and Heydon (2023) announced a 3-million-euro investment for a demonstration initiative of integrating anaerobic digestion into a green biorefining demonstration initiative.
To understand the farmer's perspective in Ireland, O'connor et al. (2021) performed a study making a survey among cattle farmers to evaluate their attitudes and readiness towards adopting anaerobic digestion (AD) technology, covering aspects such as demographics, prior experience with renewable energy, inclination towards AD adoption, preferred plant operating conditions, and perceptions regarding benefits and barriers. In the study by O'connor et al. (2021), 41 % of participants expressed willingness to adopt anaerobic digestion (AD) technology within the next five years. "Likely Adopters" had higher education levels. High costs and limited information were identified as significant barriers, while improved farm profitability was seen as a key benefit. Additionally, 58 % showed interest in a cooperative scheme, and 40.3 % preferred a self-owned and operated business model.
Park, Khim and Kim (2023) performed a study of co-digestion of pig manure with food waste, excretion, and thickened sewage sludge in a 2,775 m^3 horizontal anaerobic digester. This mixture resulted in a high yield, with a methane fraction of 68.8 % in the biogas.
Diaz Huerta et al. (2023) evaluated the utilization of biogas for boiler, CHP, upgrading and upgrading combine with CHP for farms with herd sizes of 40, 60, 100 and 185. Where the only viable scenario identified was the implementation of a boiler configuration for a herd size of 185 cows and selling the heat for district heating. O'Connor et al. (2020) evaluated the co-digestion of grass silage and dairy cow manure from farm with herd sizes of 50, 100, 150, 200 and 250 cows. The authors found that small scale anaerobic digestion is economically viable over the facility's operational lifespan, with payback periods ranging from 12.87 to 7.75 years for dairy farms with herds exceeding 100 cows, and all scenarios involving larger dairy herds showed significant net CO_2 reductions.
There are several examples of low-cost anaerobic digesters. The 15 m^3 red-mud Taiwanese PVC digester (Pound et al., 1981), a household tubular anaerobic digestion (Botero and Preston, 1987). The tubular digester can work starting with one cow for household anaerobic digestion, feeding it 20 kg of fresh manure with 60L of water and produces from 0.7 to 0.8 m^3 of biogas daily and 60L of digestate (Jaime Martí-Herrero et al., 2014). Martí-Herrero et al. (2014) provided a comprehensive overview of the results and knowledge obtained from the implementation of cost-effective tubular digesters in Bolivia over a duration of four and a half years.
To adapt this low-cost tubular digester concept to cold climate, a greenhouse concept was developed by Martí-Herrero et al. (2014a) to contain the digester in optimal temperature regimes by heating the greenhouse with solar radiation. Martí-Herrero et al. (2019) performed experiments for one year on a 13.90 m^3 low-cost reactor made with black high density polyethylene treating fruits and vegetables. This study demonstrates the technical feasibility of implementing full-scale psychrophilic anaerobic digestion (AD) for fruit and vegetable waste without the need for expensive technology, pretreatment, active heating, mixing devices, or additional water for dilution. These findings highlight the potential for the development of affordable and low-technology digesters for municipal solid waste treatment, warranting further investigation and investment.
The Canadian biodigester is a demonstrated anaerobic digester utilized mainly in pig, which consists of a covered lagoon with a digestate volume of 150m^3, made from a 0.8 mm PVC cover, and has a hydraulic retention time of around 30 days, it can treat manure from a 50-sow pig farm during a complete production cycle (Mathias, 2014). It is equipped with an internal combustion motor and a 1 mm PVC gas holder cover with a capacity of 136m^3, the biodigester efficiently processes the manure and produces biogas. The biogas is then cleaned to remove water vapor and volatile sulfides before being used for heating poultry farms, domestic applications, or grain dryers. Among the advantages of covered lagoons, their straightforward method of building, operation and maintenance provide a cost reduction (Nunes Ferraz Junior et al., 2022).
Currently in Europe, the prevailing practice involves untreated manure from agricultural fields being returned through spreading or grazing, which can have detrimental environmental effects due to nutrient excesses, imbalanced macronutrient input, and the presence of microcontaminants like metals (Rodríguez-Alegre et al., 2023). Several research studies have recognized three primary waste streams, namely manure, sewage sludge, and food processing waste, that hold potential for the production of bio-based fertilizers (Chojnacka et al., 2020). Among these waste streams, livestock manure stands as the largest, with pig slurry specifically raising significant environmental concerns regarding its safe disposal (Zhang et al., 2021). After the collection of feces and urine, these components were blended together, with the inclusion of water to achieve a solid content of 3 % dry matter, which is characteristic of swine waste (Bortoli et al., 2022).
The occurrence of inhibition is a crucial factor in anaerobic digestion (AD), and timely detection and control are necessary to prevent process failures. Inhibitory substances are defined as materials that negatively affect the microbial population or impede bacterial growth, as described by Chen, Cheng and Creamer (2008). Ammonia is the main inhibitory substance in anaerobic digestion, and its inhibitory effects are influenced by factors such as volatile fatty acid concentration, pH, temperature, the presence of other ions, and the acclimation of the anaerobic microbial community. Sulfide, produced by sulfide-reducing bacteria, can also act as an inhibitor by

competing with various anaerobic microorganisms, including hydrolytic and acetogenic bacteria, acetogens, hydrogenotrophic methanogens, and acetoclastic methanogens. Additionally, light metal ions, including aluminum, calcium, magnesium, and potassium, form another group of inhibitors in the anaerobic digestion process. Chen, Cheng and Creamer (2008) conducted a comprehensive review of the literature on the inhibition of anaerobic processes caused by both inorganic and organic substances. Their study explored the underlying mechanisms of inhibition, the factors that influence inhibition, and the common operational challenges encountered in waste treatment processes.

Anaerobic digestion encompasses three temperature ranges: psychrophilic (5 °C to 20 °C), mesophilic (30 °C to 35 °C), and thermophilic (50 °C to 60 °C). The mesophilic and thermophilic regimes are the primary options, with the mesophilic process often favoured for biogas production due to its lower energy requirements. However, it has a slower process and yields lower biogas quantities compared to the thermophilic process (Meegoda et al., 2018). To ensure optimal conditions for methanogens, the temperature control systems of anaerobic digesters should be designed to maintain a stable temperature, with a maximum deviation of ± 0.25 °C to prevent temperature fluctuations exceeding 0.5 °C (Haugen et al., 2013).

Generally, around 70 % of the methane is derived from acetate through a process involving acetoclastic methanogens. The remaining 30 % of methane is produced through the conversion of hydrogen (H_2) and carbon dioxide (CO_2), which involves hydrogenotrophic methanogens (Himanshu, 2017).

Methanogens and acetogens are frequently found in symbiotic associations, as highlighted in the study by Merlin Christy, Gopinath and Divya (2014). These microorganisms engage in simultaneous acetogenesis and methanogenesis processes, as discussed by Seadi et al. (2008), illustrating a mutually beneficial relationship between them.

A study conducted in Ireland (Wall et al., 2013) revealed that the Buswell prediction for methane production from cow slurry was 389 L CH_4/kg VS. However, according to research by Scott and Blanchard (2021), the measured biochemical methane potential (BMP) for the same slurry was 239 L CH_4/kg VS. Scott and Blanchard (2021) estimated 53 kg of manure per day, and the biomethane potential (BMP) slurry 251 L CH_4/kg VS.

Sobhi et al. (2021) proposed to utilize an air lift reactor to valorize liquid manure from open anaerobic lagoons through the recovery of nitrogen and phosphorus. By treating liquid manure at a rate of 0.5 volume of air per volume of liquid per minute for 48 hours before discharging it to anaerobic lagoons, approximately 14.5 % of TN was recovered as ammonium sulfate. Additionally, 38.8 % of TN and 79.3 % of TP were obtained as sludge, while 59.0 % of COD was eliminated. As a result, the total reduction in CH_4 and N_2O emissions was estimated to be 51.7 % less compared to traditional application methods. Sobhi et al. (2021) recommended this technology to upgrade farms that already have anaerobic lagoons.

In this study, we propose modelling the retrofitting of existing open slurry tanks into covered lagoons to harvest the biogas from the animal slurries to reduce greenhouse emissions. The digestate will be utilised as fertiliser to enhance soil health, crop yield, and productivity. Based on average herd sizes and daily slurry availability, optimal covered lagoon dimensions will be found.

2. Materials and methods

The Materials and Methods section encompasses several aspects of the anaerobic digester system design and evaluation. Initially, the study proposes a three-stage anaerobic digestion process for optimizing the digester size and efficiency. Stage 1 involves a plug flow reactor for hydrolysis and acidogenesis, followed by Stage 2, a covered lagoon where methanogenesis occurs. Stage 3 entails an open pond for storing the digestate until the spreading season. The system's conceptual design includes various components such as materials, heating systems, mixing power, and mechanisms, with options presented in an Idea Generation Matrix. Four potential configurations are identified based on the matrix's 256 combinations. Evaluations are conducted using specific criteria such as performance, economic viability, efficiency, reliability, scalability, ecological sustainability, and environmental risks. Among the options, Option 2, featuring a compacted soil digester covered with a membrane, a biogas-burning heating system, kinetic energy-driven mixing power, and an axial stirrer, is identified as the most favourable choice. The dimensions of the digester are determined based on factors such as available manure, organic loading rate, retention time, desired biogas production, and required heating. The evaluation of different farm scales, including six average Irish farms and two larger farms, provides insights into the system's performance in various scenarios. For retrofitting purposes, two specific dairy farms, Farm 1 and Farm 2, are examined, highlighting their existing infrastructure and biogas potential. Wind velocity data is also collected for both farms using the Wind Mapping System from SEAI.

2.1. Identification and planning

Traditionally, concrete digesters are utilized for anaerobic digestion, where the four steps of anaerobic digestion (hydrolysis, acidogenesis, acetogenesis, and methanogenesis) happen. To optimize the digester size, this study proposes dividing the anaerobic digestion process into three stages. Stage 1 is a plug flow reactor where the first two anaerobic digestion processes, namely, hydrolysis, and acidogenesis take place. Stage 2 is the covered lagoon where the third and fourth processes of anaerobic digestion takes place since methanogens and acetogens have syntrophic associations (Merlin Christy et al., 2014), and the biogas can be stored there for a couple of days. The third stage is an open pond, where the digestate is stored until the spreading season. Figure 54 shows these three stages in a scheme.

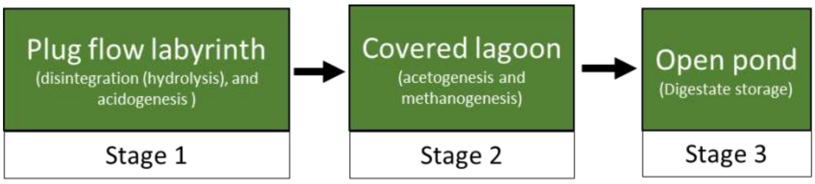

Figure 54. Proposed multistage anaerobic digester.

The manure is collected from the barn, in case any other farm wastes are to be added to the anaerobic digester, these wastes need to be pasteurized. If not, it can be directly sent to a premixing and heating pre-treatment system, then passes to a plug flow labyrinth where the first three steps of anaerobic digestion (hydrolysis, acetogenesis, and acidogenesis) take place. The is passed to a covered lagoon where the methanogenesis takes place and the biogas is produced. The next step is to dewater the digestate and send it to an open pond for storage until its spreading season. **Figure 55** shows the manure flow in the system.

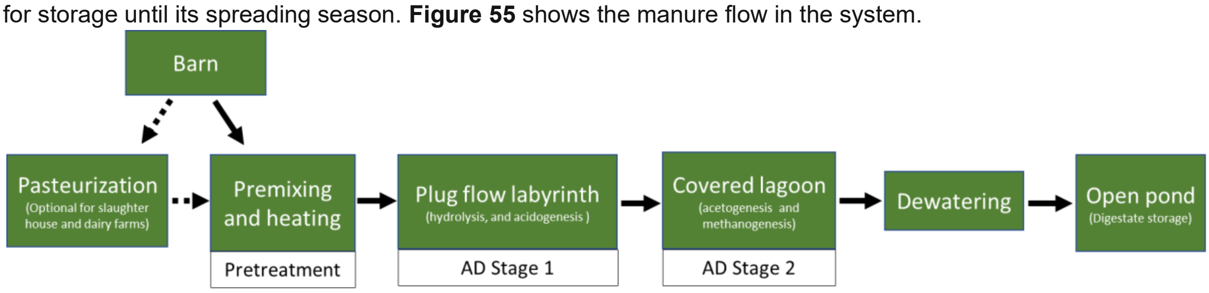

Figure 55. Manure flow in the system.

2.2. Conceptual Design: Idea Generation Matrix

The conceptual design of the anaerobic digester system involves various components such as materials, heating systems, mixing power, and mixing mechanisms. The matrix in Table 16 presents different options for each component.

Table 16. Identification and planification.

Material	Heating	Mixing power	Mixing
Concrete	Boiler	Electric motor	Transversal
Soil	Small CHP	Wind powered stirrer	Axial
Metal	Electric resistance	Combined Heat and Power (CHP)	Pump
Membrane	Solar	Small CHP per stirrer	Kinetic energy from wind

Out of the 256 possible combination, four combinations were taken as possible options for the system's configuration. The optative configurations for the system are presented in Table 17.

Table 17. Optative configurations

Configuration	Digester material	Heating system	Mixing power	Mixing
Option 1	Concrete	Burning the biogas	Combined Heat and Power	Pump
Option 2	Compacted soil covered with membrane	Burning the biogas	Kinetic energy from wind	Axial stirrer
Option 3	Soil	Electrical resistance	Small CHP per pump	Pump
Option 4	Metal	Solar mirrors array	Solar energy	Transversal

2.2.1. Systems requirements:

The anaerobic digester system should possess certain desired characteristics to ensure its effectiveness and efficiency. These characteristics may include an efficient heating system with optimal temperature control, enabling the system to maintain the ideal conditions for the anaerobic digestion process. Additionally, the system should have effective mixing power to ensure proper digestion and homogeneity of the slurry. It is also essential to use cost-effective materials that offer good durability and resistance to corrosive elements commonly found in the digestion process. Easy maintenance and operation are important aspects to consider, as they contribute to the system's reliability and longevity. Lastly, to promote sustainability, the integration of renewable energy sources into the system is desirable, reducing reliance on non-renewable energy and minimizing environmental impact.

2.2.2. Criterion Evaluation:

To evaluate the different configurations for the anaerobic digester system, several criteria were considered, including performance, economic viability, efficiency, reliability, scalability, ecological sustainability and environmental risks. These criteria were used to assess the options and determine the best choice for the system.
To evaluate the different configurations, a rating scale from 0 to 10 was used based on the following criteria:

1. Performance: This criterion assesses how well each configuration meets the heating and mixing requirements of the anaerobic digester system. The rating reflects the effectiveness and efficiency of the system in achieving optimal performance.
2. Economic Viability: The overall economic feasibility of each configuration is considered in this criterion. The rating reflects the cost-effectiveness, return on investment, and potential revenue generation of the system.
3. Efficiency: The energy efficiency of the heating and mixing mechanisms is evaluated in this criterion. The rating reflects how effectively the system utilizes energy resources, minimizing energy losses and maximizing energy conversion.
4. Reliability: The reliability and maintenance requirements of each configuration are considered. The rating assesses the system's robustness, durability, and the frequency and complexity of maintenance tasks required to ensure uninterrupted operation.
5. Scalability: The potential for the system to be scaled up or down to accommodate different farm sizes is an important consideration. The rating reflects the ease and feasibility of adjusting the system's capacity to match varying slurry volumes.
6. Ecological Sustainability: This criterion evaluates the environmental sustainability of each configuration. The rating reflects the system's impact on ecosystems, biodiversity, and natural resources, as well as its alignment with sustainable practices.
7. Environmental Risks: The potential risks and negative impacts on the environment associated with each configuration are considered in this criterion. The rating reflects the level of potential harm, pollution, or irreversible damage that could result from the system if not managed correctly.

By assigning ratings from 0 to 10 to each criterion for every configuration, a comprehensive evaluation is conducted. The option that receives the highest overall rating is considered the best choice, as it demonstrates superior performance, economic viability, efficiency, reliability, scalability, ecological sustainability, and low environmental risks compared to the other options.

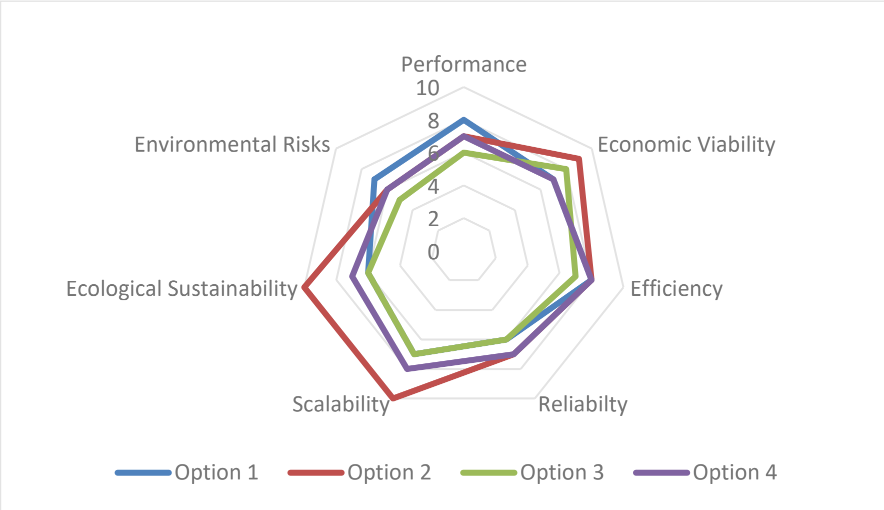

Figure 56. Attribute evaluation of different proposed configurations.

Among the evaluated options, Option 2, featuring a digester made of compacted soil covered with a membrane, a biogas-burning heating system, kinetic energy-driven mixing power, and an axial stirrer, emerged as the most favourable choice. This option demonstrated strong performance, high economic viability, good efficiency, and reliability. It also showed potential for scalability and had a positive ecological sustainability profile.

In terms of required characteristics, the anaerobic digester system aims to have an efficient heating system with optimal temperature control to ensure proper digestion. Effective mixing power is also crucial to promote homogeneity and efficient breakdown of the organic matter. Cost-effective materials with good durability and resistance to corrosive elements are desired to ensure longevity and minimize maintenance needs. Additionally, the integration of renewable energy sources, such as utilizing biogas as fuel or harnessing kinetic energy from wind, contributes to the system's sustainability and reduces environmental impact.

Considering these evaluation criteria and required characteristics, Option 2 aligns well with the goals of the anaerobic digester system. It offers a balanced combination of performance, economic viability, efficiency, reliability, scalability, and ecological sustainability. By selecting Option 2, the system can achieve efficient slurry disposal while minimizing environmental impact and ensuring long-term operational success.

2.3. Slurry disposal

The traditional approach utilized for slurry disposal is taking the manure from the barn and channelling it to an earth-lined slurry tank or slurry tower tank, until is spreading season. Open lagoons pose the challenge of high methane emissions and the potential release of toxic gases during the biological decomposition of manure in anaerobic fermentation processes (Mathias, 2014). The proposed system is utilizing a covered lagoon for capturing the biogas. **Figure 57** shows the proposed systematic transition.

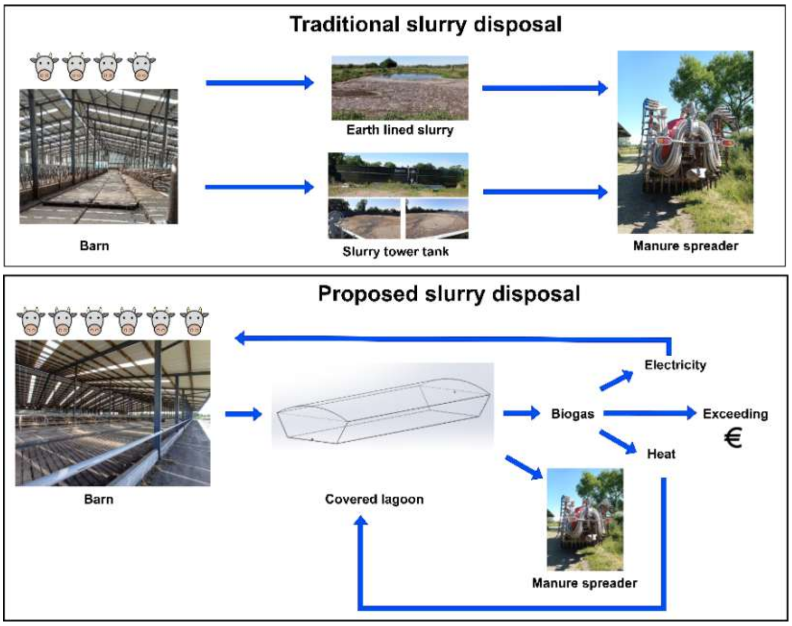

Figure 57. Proposed systematic transition

2.4. Systems dimensions

To determine the dimensions of the digester, a methodology was employed. The first step involved assessing the amount of daily available manure based on the size of the herd. This information served as the main input for the digester. To achieve the desired mix, the manure was combined with water at a ratio of 2:1. The hydraulic retention time was considered along with the organic loading rate to determine the mix of daily inputs.

Using the loading rate and retention time, the liquid volume fraction of the digester was calculated. Additionally, an estimate of the daily biogas production was derived based on these factors. This biogas production value was essential for determining the required gas volume for the digester.

The liquid volume area required for the digester was calculated separately for stage 1 (pre-treatment tank) and stage 2 (covered lagoon). Stage 2 is where biogas is generated. The calculations were based on retention times of 8-10 days for stage 1 and 15-17 days for stage 2. Once the dimensions for both stages were determined, the volume requirements for construction were established.

To meet the heating requirements, the necessary temperature for optimal anaerobic bacteria activity was considered. Ground insulation methods, such as the membrane described in the conceptual design, were utilized. A temperature control system was implemented to ensure the temperature inside the digester remained at the optimal level.

By following this methodology, the dimensions of the digester were determined based on the available manure, organic loading rate, retention time, and desired biogas production. The heating requirements were also calculated to maintain the appropriate temperature for the anaerobic bacteria's digestion process. Additionally, there is also the option to add agricultural residues.

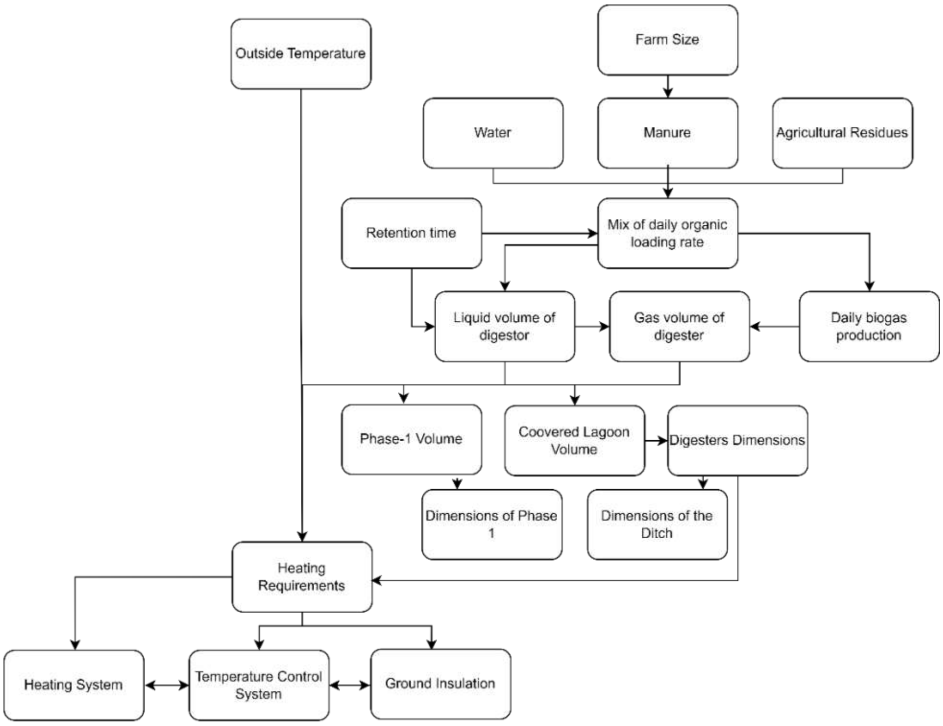

Figure 58. Methodology utilized to determine the dimensions of the systems.

2.4.1. Hydraulic retention time

The hydraulic retention time (HRT) is one of the main factors determining the size of the digester and it depends on several factors, such as the velocity of decomposition of the substrate. The HRT refers to the mean duration during which the substrate remains within the confines of the digester tank and it is influenced by both the volume of the digester and the rate at which substrate is introduced into the system (Seadi et al., 2008). The velocity and conversion rate into methane gas differ depending on the chemical composition of the substrate (Park et al., 2023).

2.4.2. Scale

For the evaluation and scale representation of the anaerobic digester system, eight farms were selected, offering a range of different scales. The first six farms were chosen from the "heavy soils program" (TEAGASC, n.d.) conducted by TEAGASC, as they provided a representative sample of the average Irish farm. These farms were selected to ensure a comprehensive understanding of the system's performance in various scenarios.
In addition to the smaller farms, two larger farms were included in the study. These farms had a herd size of 600 and 1100 cows respectively, making them larger than the average Irish farm. The purpose of including these larger farms was to propose a retrofit solution for their existing slurry disposal systems, specifically transitioning from earth-lined slurry tanks to covered lagoons. By evaluating the retrofit options for these larger farms, the study aimed to demonstrate the feasibility and benefits of implementing the covered lagoon system on a larger scale.

2.4.2.1. Average Irish farm

As an example, the “heavy soils programme” from TEAGASC (TEAGASC, n.d.) was taken to get the average herd size, soil, and air temperature for three years. This program covers 10 Irish farms, for this study only 6 farms were taken due to the herd size and location as a representation of the average Irish farm. **Figure 59** shows the locations of the six fams of the heavy soils programme.

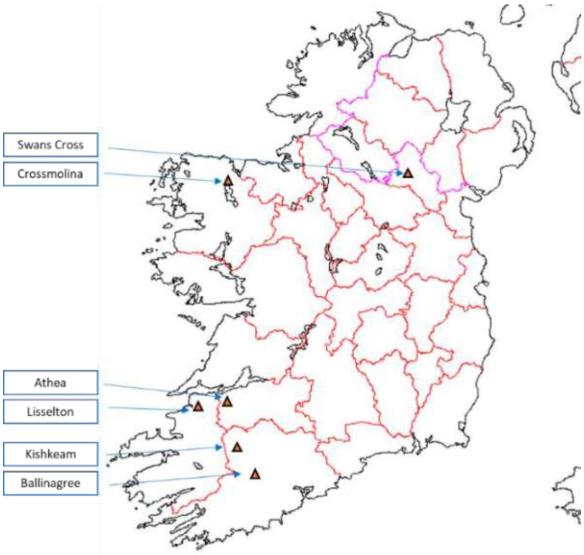

Figure 59. Map of Ireland showing the six chosen farms from the Heavy Soils program.

Table 18. Farm herd by size with an average temperature of air and soil in degrees centigrade. Data extracted from TEAGASC (2023).

Farm	Herd Size (2019)	Temperature (° C)				Potential Daily Biogas Production (m^3/d)		
		Min (Feb)		Max (July)		Min (0.35)	Average (0.385)	Max (0.42)
		Air	Soil	Air	Soil			
Crossmolina	65	3.1	4.6	16.1	16.4	54.46	59.91	65.36
Lisselton	89	4.4	5.2	16.4	15.5	74.57	82.03	89.49
Kishkeam	100	2.6	3.6	16.2	15.4	83.79	92.17	100.55
Swan Cross	110	2.7	3.7	16.2	16.5	92.17	101.39	110.60
Ballinagree	120	2.9	4.5	16	16.6	100.55	110.60	120.66
Athea	130	3.4	4.6	15.7	15.4	108.93	119.82	130.71

The data was extracted from the Wind Mapping System from SEAI (SEAI, n.d.), which is coupled with the ArcGIS World Decoding Service. This platform is Wind Atlas for Ireland, by entering the coordinates, velocity values are given for that point at different heights. The platform provides 24 datasets per day, python 3.0 was utilized to process the data, and a daily average was calculated for each farm, the values are shown in Figure **60**.

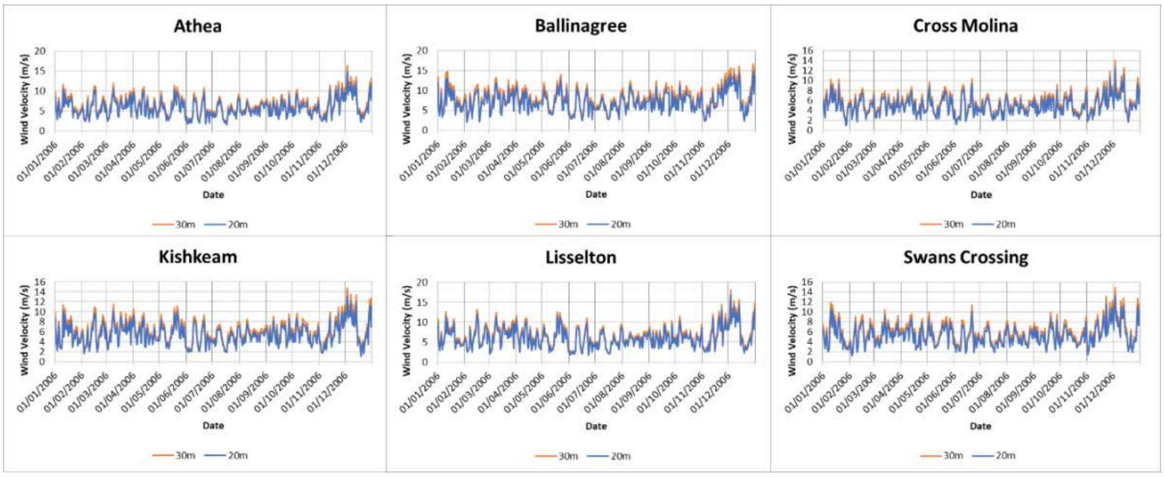

Figure 60. Average wind velocity on the six chosen farms at 20- and 30-meter heights. Data extracted from the Wind Mapping System from (SEAI, n.d.).

2.5. Dairy farms to retrofit

2.5.1. Farm 1

Farm 1 has a capacity for 1100 cows. One earth-lined slurry tank of 15 x 40 x 4 m (2,036 m^3 volume) and a slurry tower of 42 m diameter x 3 m height (4,156 m^3 volume), holding up more than 6,000 m^3. This farm has a biogas potential of 560,000 m^3/year or 1,580 m^3/d. Premixing with pump in place. The available infrastructure in farm 1 is shown in Figure 61.

Figure 61. Existing infrastructure in farm 1.

2.5.2. Farm 2

Farm 2 has a capacity for 600 cows. On the other hand, farm 2 has a capacity of 1,250 m^3 on the ELS and 640 m^3 on a second concrete storage. This farm has a biogas potential of 291,000 m^3/year or 798 m^3/d. The "barn" in this farm contains an underground tank beneath the slatted-floor cattle.
Figure 62 shows farm 2, in the center a satellite picture from the farm. Marked with green is the earth-lined slurry tank, and marked with orange is the second storage tank. The stable marked with blue has a slurry collection system with underground storage.

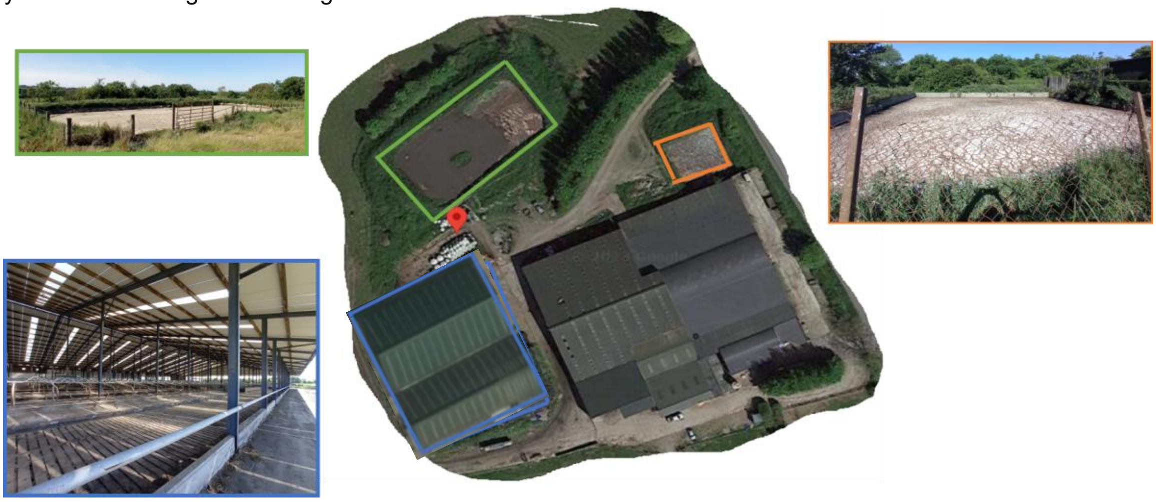

Figure 62. Existing infrastructure in farm 2.

The average wind velocity for farms 1 and 2 is shown in Figure 63 for 20 and 30 meter height.

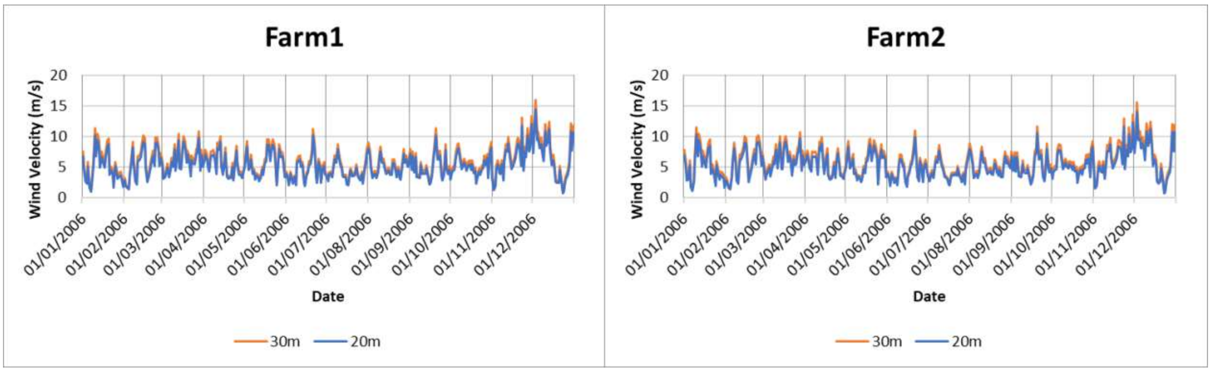

Figure 63. Average wind velocity of farms 1 and 2 at 20- and 30-meter heights. Data extracted from the Wind Mapping System from (SEAI, n.d.).

2.6. Biogas production

To calculate the biogas production per cow, we need to consider several factors. A cow generates daily from 30 to 50 kg of manure, depending on its size and diet. Within each kg of manure, there is a certain percentage of total solids. The biogas potential of every kg of manure is determined by the anaerobic digestion process, where the organic matter in the manure is broken down by microorganisms to produce biogas. The actual biogas yield per kg of manure will depend on the specific composition of the manure, including its volatile solids content and other digestible organic components. By knowing the biogas potential of each kg of manure and considering the daily amount of manure generated by a cow, we can estimate the total biogas production per cow.

3. Results and discussion

Table 19 shows the potential biogas production per farm according to their herd size.

Table 19. Potential biogas production per farm.

Farm	Herd Size (2019)	Potential Daily Biogas Production (m^3/d)		
		Min (0.35)	Average (0.385)	Max (0.42)
Crossmolina	65	54	60	65
Lisselton	89	75	82	89
Kishkeam	100	84	92.17	101
Swan Cross	110	92	101.39	111
Ballinagree	120	101	111	121
Athea	130	109	120	131
Farm 2	600	503	553	603
Farm 1	1100	922	1,014	1,106

The proposed manure life cycle is shown in Figure 64, where the manure is taken from the barn to a pre-treatment tank where it is mixed with water and preheated. Then it passes to a plug flow reactor in the form of a labyrinth where the first three anaerobic digestion processes take place. The following step is a covered lagoon where methanogenesis takes place and biogas is produced. The remaining liquid-solid fraction is called digestate, which is dewatered and sent for storage in an earth-lined slurry tank. This digestate can be utilized as fertilizer in the fields or sold for an extra income.

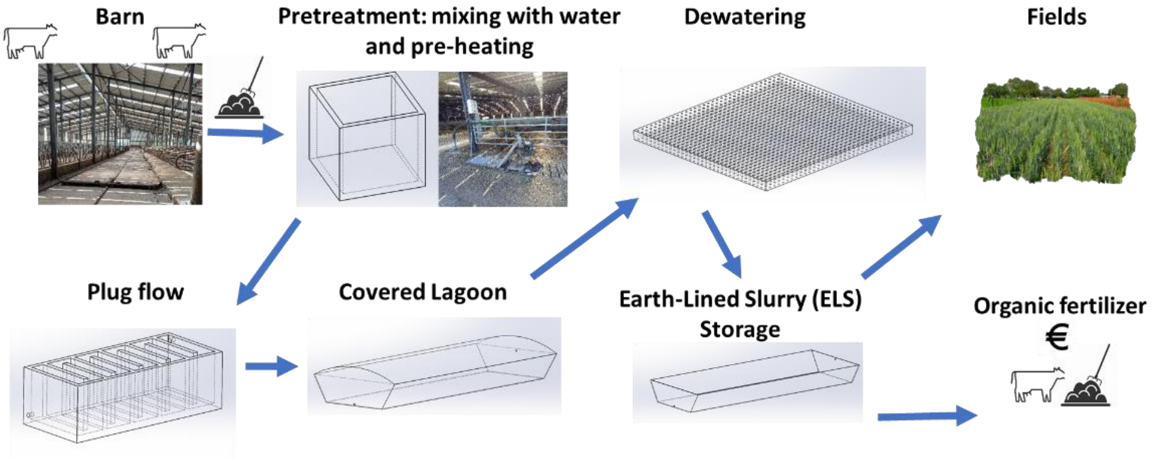

Figure 64. Resulting schematic of the proposed system.

Figure 65 shows a schematic of the heating system, the streams of water and biogas are shown with green arrows for water and yellow for the biogas. First, the biogas is extracted from the covered lagoon and passes to a biogas storage bag made from a polyethylene membrane, and then it passes through a desulphurization process to be then burned in a boiler (this is shown with yellow arrows). Water is heated up in the boiler and from there it passes first through the covered lagoon, then by the plug flow reactor (anaerobic digestion)

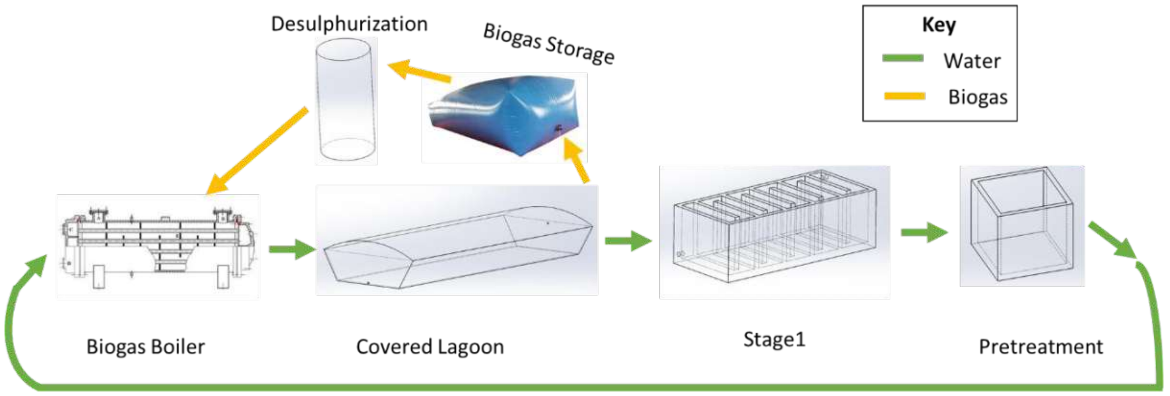

Figure 65. Water and biogas streams in the system.

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Journal Publication 7

Promoting Safe Operations in Biorefineries: A Comprehensive Safe-by-Design Framework.

Manuscript in writing in collaboration with Fernando Ramonet, Mayuki Cabrera-González, Michael Harasek.

My contribution: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Status: in writing

PROMOTING SAFE OPERATIONS IN BIOREFINERIES: A COMPREHENSIVE SAFE-BY-DESIGN FRAMEWORK

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Introduction

Safety considerations have historically been given lower priority during the initial conceptual design phase of biorefineries, with the conventional approach being to design the biorefinery first and evaluate safety aspects at a later stage (López-Molina et al., 2020).

There are eight main safe-by-design strategies. The different design methods are the probabilistic risk-based design, deterministic (safety factor-based design), fail-safe design (or fail-secure design), active safe design, passive safe design, vandal-proof design, idiot-proof (or fool-proof) design, fault-tolerant design, and circular design (van Gelder et al., 2021).

To ensure the safety of biorefineries through the "safe by design" approach, various disciplines such as biotechnology, nanomaterials, and chemical engineering are utilized. These disciplines collaborate to implement comprehensive safety measures, addressing concerns such as the containment of microorganisms, prevention of cross-contamination in feedstocks, and other potential hazards. By integrating advanced technologies and employing rigorous protocols, biorefineries can effectively mitigate risks, safeguarding both the environment and the well-being of workers. The safe-by-design approach prioritizes proactive safety considerations throughout the entire conceptual design process, ensuring that potential safety issues are identified and addressed early on to establish secure and sustainable biorefinery operations.

Materials and methods

The incorporation of safety considerations into the design process, establishes a proactive and holistic approach towards creating secure and environmentally friendly agricultural and biorefinery operations. By integrating the principles of safe by design into the conceptualization, analysis, and implementation of these sustainable practices, the research collectively seeks to optimize resource utilization, minimize environmental impact, and protect the well-being of workers, thereby paving the way for a more sustainable and resilient future.

The research approach focuses on developing a framework for safe by design in biorefineries. The objective is to shift the conventional approach, which tends to prioritize safety considerations at a later stage, by integrating safety considerations into the initial conceptual design phase. This approach aims to proactively identify and address potential safety issues, ensuring secure and sustainable biorefinery operations.

The research involves collaboration among various disciplines, including biotechnology, nanomaterials, and chemical engineering. These disciplines work together to implement comprehensive safety measures, taking into account specific concerns such as the containment of microorganisms and prevention of cross-contamination in feedstocks. By leveraging advanced technologies and employing rigorous protocols, the research aims to mitigate risks and ensure the safe operation of biorefineries.

A comprehensive framework of Safe by Design for biorefineries should include the following components:

1. Hazard Identification: Thoroughly assess potential hazards associated with biorefinery processes, including chemicals, materials, and activities that may pose risks to workers, the environment, and the surrounding community.
2. Risk and Reliability Assessment: Evaluate the likelihood, severity, and reliability of identified hazards and potential failures within the biorefinery system. Consider factors such as exposure pathways, toxicity, consequences of failures, and the overall reliability of equipment and processes.
3. Design Integration: Incorporate safety considerations into the early stages of biorefinery design, ensuring that safety features and measures are integrated into the overall process design. Consider aspects such as process layout, equipment selection, and material compatibility while prioritizing risk reduction and reliability enhancement.
4. Inherent Safety: Implement inherently safer design principles, aiming to minimize or eliminate hazards at the source rather than relying solely on protective measures. Design processes and equipment that inherently reduce the potential for accidents, such as using less hazardous materials or eliminating the need for hazardous processes.
5. Control Measures: Develop and implement engineering controls, administrative controls, and personal protective measures to mitigate identified risks. This may include ventilation systems, containment systems, safety interlocks, standard operating procedures, training programs, and personal protective equipment.
6. Monitoring, Maintenance, and Reliability Management: Establish a comprehensive monitoring and maintenance program to continuously assess the performance, reliability, and safety of the biorefinery system. Regular inspections, preventive maintenance, reliability-centred maintenance, and equipment reliability assessments are essential to ensure ongoing safety and minimize the risk of failures.
7. Emergency Preparedness: Develop emergency response plans and procedures to effectively handle potential incidents or accidents. This includes establishing communication protocols, training personnel on emergency response, conducting drills, and ensuring the availability of appropriate emergency equipment and resources.
8. Compliance and Auditing: Regularly evaluate and audit the biorefinery's safety practices to ensure compliance with relevant regulations, standards, and best practices. Identify areas for improvement and ensure continuous adherence to safety protocols through internal audits and external assessments.
9. Communication and Training: Ensure effective communication of safety policies, procedures, and expectations to all stakeholders, including workers, contractors, and neighbouring communities. Regular training programs should be conducted to enhance safety awareness, promote a culture of safety, and provide specific training on handling hazardous materials and operating equipment safely.
10. Continuous Improvement and Total Quality Management: Foster a culture of continuous improvement by implementing principles from Total Quality Management and lean manufacturing methodologies. Encourage employee involvement in identifying safety improvement opportunities, implementing corrective actions, and promoting a proactive approach to safety and reliability enhancement.

By incorporating these elements, a comprehensive framework of Safe by Design for biorefineries can help identify and mitigate potential hazards, ensure the safety of workers and surrounding communities, enhance system reliability, and promote the sustainable and responsible operation of biorefinery processes.

The research approach entails the identification and evaluation of different safe-by-design strategies. These strategies include probabilistic risk-based design, deterministic (safety factor-based) design, fail-safe design, active safe design, passive safe design, vandal-proof design, idiot-proof (or fool-proof) design, fault-tolerant design, and circular design. Through a comprehensive analysis of these strategies, the research aims to determine the most effective approaches for integrating safety considerations into the conceptual design process of biorefineries.

Overall, the research approach for Journal Publication 7 encompasses the development of a comprehensive framework for safe by design in biorefineries. Through interdisciplinary collaboration, the integration of advanced technologies, and the evaluation of different safe-by-design strategies, the research aims to prioritize safety considerations from the early stages of conceptual design, thereby establishing secure and sustainable biorefinery operations.

Results

The safe by design framework represents a comprehensive approach to ensure the safety, environmental responsibility, and reliability of biorefinery operations. It encompasses various stages and interconnected elements that work together to minimize risks, protect the environment, and promote secure and sustainable practices. Figure 1 illustrates an integrated framework for safe by design in biorefineries, emphasizing the interdependence of key elements in ensuring the safety and reliability of biorefinery processes.

The framework begins with hazard identification, where potential risks associated with biorefinery processes are thoroughly assessed. This is followed by risk and reliability assessment, evaluating the likelihood and severity of identified hazards. Design integration plays a crucial role by integrating safety considerations into the early stages of biorefinery design, ensuring that safety features and measures are incorporated from the beginning. Inherent safety principles aim to minimize hazards at their source, while control measures are implemented to mitigate risks throughout the operations. Monitoring, maintenance, and reliability management are vital components of the framework, ensuring ongoing safety and performance of the biorefinery system. Emergency preparedness plans and procedures are developed to effectively handle potential incidents or accidents. Compliance and auditing practices ensure adherence to safety protocols, regulations, and standards. Continuous improvement is promoted through effective communication, comprehensive training programs, and total quality management principles.

Figure 1 illustrates an integrated framework for safe by design in biorefineries. The central circle represents the biorefinery system, while eight outer circles represent key elements of the framework. The figure emphasizes the interconnectedness and interdependence of these elements in ensuring the safety and reliability of biorefinery operations. The framework encompasses various stages, starting with hazard identification, where potential risks associated with biorefinery processes are thoroughly assessed. Risk and reliability assessment evaluate the likelihood and severity of identified hazards, while design integration integrates safety considerations into the early stages of biorefinery design. Inherent safety principles aim to minimize hazards at their source, and control measures are implemented to mitigate risks. Monitoring, maintenance, and reliability management ensure ongoing safety and performance, while emergency preparedness addresses potential incidents or accidents. Compliance and auditing ensure adherence to safety protocols, and the framework promotes continuous improvement through communication, training, and total quality management. The figure visually represents the comprehensive approach to safe by design, highlighting the importance of integrating safety measures across all aspects of biorefinery operations.

Figure 1. Integrated Framework for Safe by Design in Biorefineries.

Figure 2 represents the comprehensive framework for safe by design in biorefineries, visualized in the form of an onion with layers. At the centre of the figure, we find the human element, symbolizing the utmost importance of ensuring the safety and well-being of workers and surrounding communities throughout the biorefinery processes. Moving outward, the second layer focuses on implementing robust safety measures in biotechnology to prevent the release of genetically modified organisms and microorganisms outside the facility. The third layer emphasizes the need to maintain the integrity of feedstock materials and prevent cross-contamination along the production processes. The fourth layer highlights the significance of environmental considerations, promoting practices that minimize the environmental impact of biorefinery operations. Lastly, the outermost layer represents the reliability of processes, emphasizing the importance of robust design, quality control, and regular maintenance to ensure consistent and predictable performance. Together, these layered elements form a holistic framework that prioritizes safety, environmental responsibility, and reliability in the design and operation of biorefineries, promoting secure and sustainable practices in this important field.

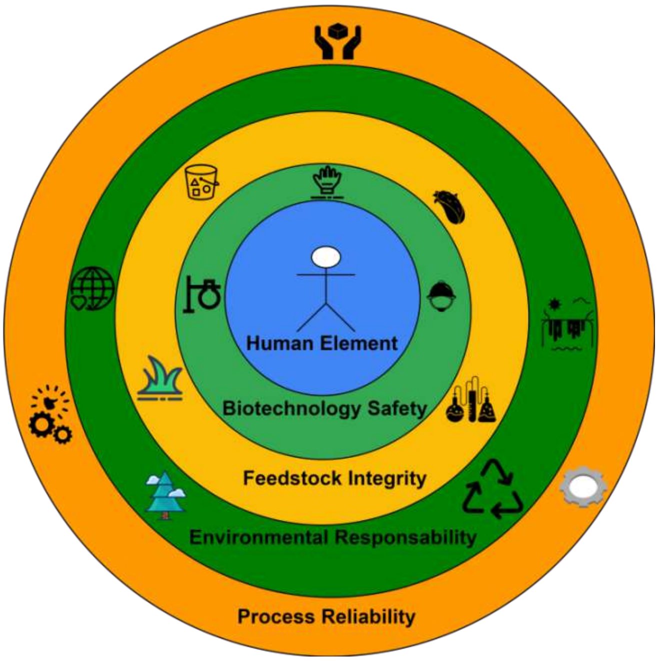

Figure 2. Comprehensive Framework for Safe by Design in Biorefineries: Layered Approach for Safety, Environmental Responsibility, and Reliability

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Conference publications

Conference Publication 1

Modelling of Multi-Stage Internal Loop Air Lift Bioreactor Utilizing Computational Fluid Dynamics

My contributions: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Ramonet, F., Haddadi, B, Harasek, M., (2023), Modelling of Multi-Stage Internal Loop Air Lift Bioreactor Utilizing Computational Fluid Dynamics, 17th Minisymposium Verfahrenstechnik and 8th Partikelforum, BOKU, Vienna, April 13th – 14th, 2023 ISBN: 978-3-900397-08-1

Conference Poster 1

Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions

My contributions: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Mayuki Cabrera-González, Fernando Ramonet, Michael Harasek. Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions. Circular@WUR: Living within planetary boundaries, Wageningen University and Research, Wageningen, 11-13 April, 2022. DOI: 10.13140/RG.2.2.21658.11200

Conference Poster 2

Study on the Co-Digestion of Nopal Cladodes with Farm Manures

My contributions: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Fernando Ramonet, Michael Harasek. Modelling Study on the Co-Digestion of Nopal Cladodes with Farm Manures. 30th European Biomass Conference & Exhibition (EUBCE2022). Paris, France (online), 9-12 May, 2022, ISBN: 978-88-89407

Conference Poster 3

Modelling And Characterization Of Internal Loop Air Lift Bioreactor Configurations Through Computational Fluid Dynamics

My contributions: Conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualisation.

Fernando Ramonet, Bahram Haddadi, Michael Harasek. Modelling And Characterization Of Internal Loop Air Lift Bioreactor Configurations Through Computational Fluid Dynamics. Biorefine Conference 'The role of biorefineries in European agriculture'. Ghent, Belgium, 30-31 May, 2022. DOI: 10.13140/RG.2.2.16383.89765

Public report 1

State-of-the-art Report on Anaerobic Digestion and Biorefinery Systems Level Design

My contributions: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization.

Srija Balachandran, Mariana Cerca, Rushab Chopda, Fernando Ramonet, Charlene Vance, Steven De Meester, Michael Harasek Erik Meers, Fionnuala Murphy, Ana Robles-Aguilar. State-of-the-art Report on Anaerobic Digestion and Biorefinery Systems Level Design. European Comission. Reference Ares(2021)2235935 - 31/03/2021.

Report available at:

- Community Research and Development Information Service (CORDIS): https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5db4cee55&appId=PPGMS
- ResearchGate: https://www.researchgate.net/publication/368789796_Chapter_three_Three-Phase_Bioreactor_Scalability_and_Anaerobic_Digestion_Retrofitting_Analysis

Public report 2

CFD optimisation and analysis of existing AD and Biorefineries Report

My contributions: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization.

Fernando Ramonet, Michael Harasek. CFD optimisation and analysis of existing AD and Biorefineries Report. European Comission. Reference Ares(2021)7353824 - 29/11/2021.

Report available at:

- Community Research and Development Information Service (CORDIS): https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5e52d5093&appId=PPGMS
- ResearchGate: https://www.researchgate.net/publication/367500195_Computational_Fluid_Dynamics_optimisation_and_analysis_of_existing_Anaerobic_Digestion_and_Biorefineries_Report

Public report 3

Geometry and CFD results for AD retrofit and TPB up scaling Report

My contributions: conceptualization, methodology, validation, formal analysis, investigation, writing—original draft preparation, writing—review and editing, visualization.

Fernando Ramonet, Michael Harasek. Geometry and CFD results for AD retrofit and TPB up scaling Report. European Commission. Submitted on February 7, 2023.

Once the report submitted to the European Commission has been accepted, it will be published on: https://cordis.europa.eu/project/id/860477/results

The code is available for download at: https://github.com/AgRefineESR10/Deliverable-D2.5

Curriculum Vitae

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Education
Bachelor:
Bachelor´s Degree in Industrial and Systems Engineer.
In University of Sonora (2011-2016), Mexico.

Postgraduate:
Master's Degree in Mechanical Engineering.
At Technical University of Madrid (2018-2020), Spain.
Master´s Thesis: Design, Manufacture, Assembly and Synchronization of a Mechanical System for the Tomographic Inspection Through Ultrasounds.
Institution: Spanish Council for Scientific Research (CSIC).

Ph.D. in Chemical Engineering.
At Vienna University of Technology (2020-2023), Austria.
Ph.D. Thesis: Circular Bioeconomy Applications in Chemical Engineering.

Languages:
Spanish: Native
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Professional Experience
EARLY-STAGE RESEARCHER (PHD RESEARCHER) 2020- ONGOING
Project´s name: AgRefine
Company: Vienna University of Technology (TU Wien)
Predoctoral researcher, PhD in chemical engineering.
Retrofitting of biogas plants for integration into biorefineries through computational fluid mechanics and process simulation.

CONSULTANT 2018-ONGOING
Engineering Technical Advisor for companies in the metal-mechanic industry.
Companies: Fábricas Ramonet SA De CV and R. Bravo SA De CV.
Design of components, instructions, and drawings for manufacturing.

Development of manufacturing and inspection procedures manuals according to national and international standards.
Development and validation of procedures for Non-Destructive Testing.
Training of personnel in industrial ultrasound, thickness measurement, visual inspection, liquid penetrant, magnetic particle, spark testing and hydrostatic pressure testing.

VISITING RESEARCH FELLOW **2022**
Company: Enviroeye Engineering Ltd.
Place: Dublin, Ireland
Duration: Three months

INTERNSHIP **2018-2019**
Project Name: Technical Assistant
Entity: Spanish Association of Air Conditioning Equipment Manufacturers (AFEC).
Place: Madrid, Spain.
Technical Analyses, European Guides Translations, technical team support.
Duration: Six Months

FABRICAS RAMONET S.A. DE C.V. **2013- 2018**
Executed Non-Destructive Examinations in Welding and in Pressure Vessels.
Designed, Developed and Implemented Quality and Maintenance Programs.
Designed and Developed Manuals Procedures for Non-Destructive Testing.
Generated Project Quotations.
Duration: 4 years, 10 months, 20 days.

INTERNSHIP **2015**
Projects name: Development of Non-Destructive Testing Procedures Manuals in Fabricas Ramonet S.A. De C.V.
Developed self-ability to analyze and interpret standards and codes.
Duration: Six Months.

SOCIAL SERVICE **2015**
Center of Metrology Assistance of the University of Sonora.
Precision Measuring and Uncertainty Analyses.
Calibration of Measuring Instruments.
Duration: Six Months.

Courses and certifications

1. Course name: Liquid Penetrant Testing Level I & II
   Date: 5 to 7 of August 2014
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   Entity: LLOGSA
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   Date: 2 to 4 de May 2023
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   Entity: LLOGSA

Duration: 24 hours

3. Course name: Visual Testing Level I &II
Date: 1 to 3 of July 2014
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4. Course name: Visual Testing Level I &II
Date: 21 to 23 March 2023
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5. Course name: Ultrasonic Testing Level I
Date: 12 to 16 of August 2013
Place: Mexico City, Mexico.
Entity: LLOGSA
Duration: 40 hours
6. Course name: Ultrasonic Testing Level II
Date: 2 to 6 of September 2013
Place: Mexico City, Mexico.
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7. Course name: Ultrasonic Testing Level II
Date: 24 to 28 of April 2017
Place: Mexico City, Mexico.
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Duration: 40 hours
8. Course name: Ultrasonic Testing Level II
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Duration: 40 hours
9. Course name: Magnetic Particle Testing Level I & II
Date: 6 to 8 of May 2014
Place: Mexico City, Mexico
Entity: LLOGSA
Duration: 24 hours
10. Course name: Magnetic Particle Testing Level I & II
Date: 21 to 24 February 2023
Place: Online.
Entity: LLOGSA
Duration: 32 hours
11. Course name: Radiographic Testing Level I
Date: 13 to 17 of April 2015
Place: Mexico City, Mexico
Entity: LLOGSA
Duration: 40 hours
12. Course name: Metallographic Analysis
Date: 5 to 8 of January 2016

Place: Hermosillo, Mexico.
Entity: University of Sonora
Duration: 20 hours

13. Course name: Introduction to Mechanical Design in SolidWorks
    Date: 6 to 24 of April 2015
    Place: Hermosillo, Mexico.
    Entity: University of Sonora
    Duration: 40 hours
14. Certification name: Green Belt in Six Sigma Methodology
    Date: 17 of August to 27 of November 2015
    Place: Hermosillo, Mexico.
    Entity: University of Sonora
    Duration: 70 hours
15. Course name: Geometric Dimensions and Tolerances (GD&T) - ASME Y14.5M
    Date: July 2020
    Place: Udemy
    Entity: Udemy
    Duration: 7 hours
16. Course name: Industrial Biotechnology
    Date: 20 December 2020
    Place: Coursera
    Entity: University of Manchester
    Duration: 6 Weeks
17. Course name: Introduction to Algae
    Date: 11 January 2021
    Place: Coursera
    Entity: University of California San Diego
    Duration: 5 Weeks
18. Course name: Responsible Research and Innovation
    Date: 12 to 19 January 2022
    Place: Online
    Entity: Wageningen University & Research
    Duration: 30 hours
19. Course name: TWi Technical Writing Skills
    Date: 15 to 16 March 2022
    Place: Cork, Ireland
    Entity: TECHNICALLY WRITE IT
    Duration: 16 hours
20. Course name: High-Performance Computing in Engineering with a focus on Computational Fluid Dynamics
    Date: 12 to 16 September 2022
    Place: Bologna, Italy
    Entity: SC Train Consortium, CINECA
    Duration: 32 hours
21. Course name: Safe by Design
    Date: 7 to 9 June 2023
    Place: The Hague, Netherlands
    Entity: TU Delft

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Awards and Degree Evaluations

I. Award: I have a Non-Destructive Testing Project (Spanish: "Tengo un Proyecto de END")
Category: Special Mention for best NDT Master's Thesis
Entity: Spanish Association of Non-Destructive Testing (AEND) and the Spanish National Research Council (CSIC)
Date: 24 November 2021

II. Grant: Marie Skłodowska-Curie Grant Agreement No 860477
Duration: September 2020 to September 2023
Entity: European Commission

III. Evaluation´s Name: National Examination for Bachelor Graduation in Industrial Engineering.
Date: 14 August 2015
Place: Hermosillo, Mexico
Entity: The Higher Education National Assessment Center C.A.
Duration: 8 hours
Grade: Outstanding

IV. Evaluation´s Name: Presentation of Master´s Degree Thesis
Thesis Name: Design, manufacture, assembly, and synchronization of a mechanical system for the tomographic inspection by ultrasounds.
Date: 25 February 2020
Place: Madrid, Spain
Entity: Technical University of Madrid
Duration: 30 Minutes
Grade: 9.9 (Honors)

Publications

1. Title: Diseño, Fabricación, Ensamble Y Sincronización De Un Sistema Mecánico Para La Inspección Tomográfica Por Ultrasonidos
Type: Technical article
Journal: Revista Asociación Española de Ensayos No Destructivos
Vol. 98, Pag 40-47,
ISSN: 1888-9166
Date: 5 April 2022
2. Title: Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions
Type: Scientific article
Journal: Land MDPI
Vol. 11, Issue 9, Pag 1-17
DOI: https://doi.org/10.3390/land11091506
Date: 7 September 2022
3. Title: Modelling and Design of Optimal Internal Loop Air-Lift Reactor Configurations Through Computational Fluid Dynamics
Type: Scientific article
Journal: Chemical Engineering Transactions

Vol. 94, Pag 817-822
DOI: https://doi.org/10.3303/CET2294136
Date: 1 September 2022

4. Title: Anaerobic Digestion as a Carbon Capture, Storage, and Utilization Technology
Type: Scientific article
Journal: Chemical Engineering Transactions
Vol. 96, Pag 49-54
DOI: https://doi.org/10.3303/CET2296009
Date: 30 November 2022
5. Title: Optimal Design of Double Stage Internal Loop Air-Lift Bioreactor

   Type: Scientific article
   Journal: Energies MDPI
   Vol. 16, Issue 7, Pag 1-21
   DOI: https://doi.org/10.3390/en16073267
   Date: 6 April 2023
6. Title: Bioreactor Mixing: A Comparison of Computational Fluid Dynamics and Experimental Approaches in the Pursuit of Sustainable Bioprocessing for the Bioeconomy

   Type: Scientific article
   Journal: Chemical Engineering Transactions
   Submitted: June 2023
7. Title: Desarrollo De Manuales De Pruebas No Destructivas En Fabricas Ramonet S.A. De C.V., Reporte Técnico Final de Prácticas Profesionales

   Type: Report
   Entity: Fabricas Ramonet S.A. de C.V. y Universidad de Sonora
   Pag 1-152
   Date: 10 January 2016
8. Title: Diseño, fabricación, ensamble y sincronización de un sistema mecánico para la inspección tomográfica por ultrasonidos

   Type: Master's Thesis
   Entity: Technical University of Madrid (Universidad Politécnica de Madrid)
   Pag 1-159
   Date: January 2020
9. Title: State of the art report on AD and biorefinery system levels design

   Type: Report
   Entity: European Commission
   Pag 20-44
   Date: 31 March 2021
   https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5db4cee55&appId=PPGMS
10. Title: CFD optimisation and analysis of existing AD and Biorefineries

    Type: Report
    Entity: European Commission
    Pag 1-99
    Date: 29 November 2021
    https://ec.europa.eu/research/participants/documents/downloadPublic?documentIds=080166e5e52d5093&appId=PPGMS
11. Title: Geometry and CFD results for AD-retrofit and TPB-up-scaling Report

Type: Report
Entity: European Commission
Pag 1-88
Date: 7 February 2023

Workshops

1. Workshop name: Lean Manufacturing Workshop

   Date: 12 of April 2013
   Place: Hermosillo, Mexico.
   Entity: University of Sonora
   Duration: 3 hours

Conferences

1. 13th International Simposium on Engineering Axis 2013 Proyecta

   Participation: Assistant
   Date: 9 to 12 of April 2013
   Place: Hermosillo, Mexico.
   Entity: University of Sonora
2. 1st International Congress on Embedded Software and Mechatronics
   Participation: Assistant Date: 30 of October to 1 of November 2014
   Place: Juriquilla, Mexico.
   Entity: Mexican Association of Embedded Software
3. 14th National Congress of the Mexican Association of Mechatronics AC
   Participation: Organizing Committee
   Date: 15 to 17 of October 2015
   Place: Juriquilla, Mexico.
   Entity: Mexican Association of Mechatronics AC
4. Circular@WUR: "Living within planetary boundaries"
   Participation: Presenter (poster)
   Poster Title: Development of a Model for the Implementation of the Circular Economy in Desert Coastal Regions
   Date: 11 to 13 de April 2022
   Place: Wageningen, Netherlands.
   Entity: Wageningen University & Research
5. 30th European Biomass Conference and Exhibition (EUBCE2022)
   Participation: Presenter (poster)
   Poster Title: Modelling Study on the Co-Digestion of Nopal Cladodes with Farm Manures
   Date: 9 to 12 de May 2022
   Place: Online
   Entity: ETA Florence Renewable Energies
6. Biorefine Conference: "The role of biorefineries in European agriculture "
   Participation: Presenter (poster)
   Poster Title: Modelling And Characterization Of Internal Loop Air Lift Bioreactor Configurations Through Computational Fluid Dynamics
   Date: 30 to 31 May 2022

Place: Ghent, Belgium.
Entity: Gent University and Biorefine Cluster

7. 25th Conference on Process Integration for Energy Saving and Pollution Reduction – (PRES'22)
   Participation: Presenter (oral presentation)
   Title: Modelling and Design of Optimal Internal Loop Air-Lift Reactor Configurations Through Computational Fluid Dynamics
   Date: 5 to 8 September 2022
   Place: Bol, Croatia.
8. 1st International Conference On Energy, Environment & Digital Transition (E2DT)
   Participation: Presenter (oral presentation)
   Title: Anaerobic Digestion as a Carbon Capture, Storage, and Utilization Technology
   Date: 24 to 26 October 2022
   Place: Milan, Italia.
9. I Congreso Internacional de Biotecnología Ambiental y Economía Circular, Lima, Peru.
   Participation: Presenter (Keynote Speaker)
   Title: Aplicaciones Y Desarrollo De La Economía Circular
   Date: 6 to 7 December 2022
   Place: Cesar Vallejo University in Lima, Peru y online.
10. Universidad de Sonora, Departamento de Ingeniería Industrial
    Participation: Presenter (Keynote Speaker)
    Title: Diseño, Fabricación, Ensamble Y Sincronización De Un Sistema Mecánico Para La Inspección Tomográfica Por Ultrasonido
    Date: 14 March 2023
    Place: Universidad de Sonora in Hermosillo, Mexico.
11. 7th Minisymposium Verfahrenstechnik and the 8th Partikelforum
    Participation: Presenter (oral presentation)
    Title: Modelling of Multi-Stage Internal Loop Air Lift Bioreactor Utilizing Computational Fluid Dynamics
    Date: 13 April 2023
    Place: University of Natural Resources and Life Sciences, Vienna (BOKU) in Vienna, Austria.